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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Package for PANEL: CRA-2014 Performance Assessment

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Acronyms

AP	Analysis Plan
CCA	Compliance Certification Application
CFR	Code of Federal Regulations
CH	Contact Handled
CMS	Configuration Management System
CRA	Compliance Recertification Application
DBR	Direct Brine Release
DCL	Digital Command Language
DOE	US Department of Energy
DRZ	Disturbed Rock Zone
EPA	Environmental Protection Agency
ERDA	Energy Research and Development Administration
FMT	Fracture-Matrix Transport
GWB	Generic Weep Brine
LANL	Los Alamos National Laboratory
LHS	Latin Hypercube Sampling
PA	Performance Assessment
PABC	Performance Assessment Baseline Calculation
PAPDB	Performance Assessment Parameter Database
PAVT	Performance Assessment Verification Test
PC	Personal Computer
POD	Parameter Output Database
RH	Remote Handled
SNL	Sandia National laboratories
TRU	Transuranic
WIPP	Waste Isolation Pilot Plant

1. INTRODUCTION

1.1 BACKGROUND

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models used in PA are maintained and updated with new information as part of an ongoing process. Improved information regarding important WIPP features, events, and processes typically results in refinements and modifications to PA models and the parameters used in them. Planned changes to the repository and/or the components therein also result in updates to WIPP PA models. WIPP PA models are used to support the repository recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

PA calculations were included in the 1996 Compliance Certification Application (CCA) (U.S. DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT) (MacKinnon and Freeze 1997a, 1997b and 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the regulatory containment criteria. The facility was approved for disposal of transuranic waste in May 1998 (U.S. EPA 1998). PA calculations were an integral part of the 2004 Compliance Recertification Application (CRA-2004) (U.S. DOE 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC) (Leigh et al. 2005), be conducted with modified assumptions and parameter values (Cotsworth 2005). Following review of the CRA-2004 and the CRA-2004 PABC, the EPA recertified the WIPP in March 2006 (U.S. EPA 2006).

PA calculations were completed for the second WIPP recertification and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). To incorporate additional information which was received after the CRA-2009 PA was completed, but before the submittal of the CRA-2009, the EPA requested an additional PA calculation, referred to as the 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al. 2010), be undertaken which included updated information (Cotsworth 2009). Following the completion and submission of the PABC-2009, the WIPP was recertified in 2010 (U.S. EPA 2010).

The Land Withdrawal Act (U.S. Congress 1992) requires that the DOE apply for WIPP recertification every five years following the initial 1999 waste shipment. The 2014 Compliance

Recertification Application (CRA-2014) is the third WIPP recertification application submitted by the DOE for EPA approval. The PA executed by SNL in support of the CRA-2014 is detailed in AP-164 (Camphouse 2013). The CRA-2014 PA includes a number of technical changes and parameter refinements, as well as a redesigned WIPP panel closure system. Results found in the CRA-2014 PA are compared to those obtained in the PABC-2009 in order to assess repository performance in terms of the current regulatory baseline. This analysis package documents the actinide mobilization assessments of the CRA-2014 PA PANEL analysis.

1.2 OBJECTIVES FOR THE CRA-2014 PA PANEL ANALYSIS

Several changes are incorporated in the CRA-2014 PA relative to the CRA-2009 PABC. The modifications include repository planned changes, parameter updates, and refinements to PA implementation (Camphouse 2013). The issues and changes affecting the PANEL portion of WIPP PA include the following:

1) Actinide solubilities were updated.
2) Implementation of uncertainty for the actinide solubilities was updated.
3) Inventory information was updated.
4) Multiple brine volumes were implemented.

2. CHANGES FROM THE CRA-2009 PABC TO THE CRA-2014 PA THAT AFFECT PANEL CALCULATIONS

2.1 ACTINIDE SOLUBILITY UPDATE

Brush and Domski (2013a) and Brush (2013) provided the new baseline solubilities of Th(IV), Np(V), and Am(III) for the CRA-2014 PA. The WIPP Th(IV), Np(V), and Am(III) thermodynamic speciation and solubility models, implemented in **EQ3/6**, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010, Xiong, 2011b), and the thermodynamic database (DB) **DATA0.FMT.R2**, known as **DATA0.FM1** (Xiong, 2011a), were used to calculate the solubilities of actinide (An) elements in the +III, +IV, and +V oxidation states, respectively, in WIPP brines under expected near-field chemical conditions.

Prediction of the long-term near-field chemical conditions expected in WIPP disposal rooms comprised: (1) use of WIPP-relevant standard brines with five different volumes to simulate fluids that could enter the repository. In particular GWB brine (Generic Weep Brine), which represents brine that could enter the repository from the Salado Formation, and ERDA-6 brine (Energy Research and Development Administration), which represents brine that could enter the repository from the Castile Formation; (2) the assumption that instantaneous, reversible equilibria among these brines, major Salado minerals, and MgO hydration and carbonation products will control chemical conditions; and (3) use of a thermodynamic model in the speciation and solubility code **EQ3/6** to calculate these chemical conditions. Brush et al. (2012a, 2012b) described these assumptions, brines, and methods in detail.

Predictions of An(III), An(IV)m, and An(V) solubilities involved: (1) use of speciation and solubility models for Th(IV), Np(V), and Am(III); (2) use of WIPP-relevant standard brines that are 1 ×, 2 ×, 3 ×, 4 ×, and 5 × 17,400 m^3 (Brush, Domski and Xiong, 2012b), to simulate fluids

that could enter the repository. ; (3) use of **EQ3/6** to calculate the solubilities of Th(IV), Np(V), and Am(III); (4) use of the current thermodynamic database, **DATA0.FM1** (Xiong, 2011a); (5) use of uncertainty ranges and probability distributions for the Th(IV), Np(V), and Am(III) solubility predictions (Brush and Domski, 2013b); (6) predictions of the redox speciation of Th, U, Np, Pu, and Am under the near-field chemical conditions expected in the WIPP; (7) use of the oxidation-state analogy to apply the solubilities calculated for Th(IV), Np(V), and Am(III) to other actinides in the WIPP; and (8) use of a solubility estimate for U(VI) (see below). Brush and Domski (2013a) discussed the predictions of actinide solubilities in detail.

Most of the assumptions, brines, databases, and methods used to predict near-field chemical conditions and the solubilities of Th(IV), Np(V), and Am(III) for the CRA-2014 PA (Brush and Domski, 2013a) were identical to those used by Brush et al. (Brush, Domski and Xiong, 2012b).

Camphouse (Camphouse, 2013) indicated that the CRA-2014 PA includes planned changes as well as parameter and implementation changes. In the CRA-2014 PA, a number of individual cases were investigated the isolated impact associated with each change, as well as the combined impact when all changes are included in the PA. PANEL outputs are impacted by a baseline (BL) set of changes, where the brine volume changes are not implemented. Some of the changes considered in BL case (CRA14-BL) are (Camphouse, 2013): (1) updates of inventory parameters including colloid parameters, and (2) radionuclide solubility updates and their uncertainty updates, with the minimum brine volume (17,400 m^3). The impact of the variable brine volume (BV) implementation is assessed for case CRA14-BV. Cases BL and BV include only replicate 1. Case CRA14-0 incorporates all changes in three replicates. Results from case CRA14-0 are compared to those from the CRA-2009 PABC. In this way, this analysis provides PANEL results with five variable brine volumes: BVk = k × 17,400 m^3 (k = 1, 2, 3, 4, 5).

Actinide solubilities calculated by **EQ3/6** are represented in the remainder of this document as:

$$\left(s_{brine}^{red/ox}\right) \tag{1}$$

and are defined for a particular actinide oxidation state (+III, +IV, +V, +VI) and brine (Salado or Castile). Table 1 provides the An(III), An(IV), and An(III) solubilities at various brine volumes (BVk = k × 17,400 m^3, k = 1, 2, 3, 4, 5) established for the CRA-2014 PA (Brush, 2013) and compares them to those established for the CRA-2009 PABC (Brush and Xiong, 2009c). Table 2 provides a list of the solubility uncertainty values.

Table 1. Actinide-Solubility Parameters Used for the CRA-2009 PABC and the CRA-2014 PA[(a)]

Material	Property	Description	CRA-2009 PABC	CRA-2014 PA BV1	CRA-2014 PA BV2	CRA-2014 PA BV3	CRA-2014 PA BV4	CRA-2014 PA BV5	Units
SOLMOD3	SOLCOH	Solubility of +III actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	1.51E-06	1.48E-06	8.59E-07	5.99E-07	4.69E-7	3.92E-07	moles/liter
	SOLSOH	Solubility of +III actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	1.66E-06	2.59E-06	1.38E-06	9.74E-07	7.69E-07	6.47E-07	moles/liter
SOLMOD4	SOLCOH	Solubility of +IV actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	6.98E-08	7.02E-08	7.14E-08	7.17E-08	7.19E-08	7.20E-08	moles/liter
	SOLSOH	Solubility of +IV actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	5.63E-08	6.05E-08	6.06E-08	6.07E-08	6.07E-08	6.07E-08	moles/liter
SOLMOD5	SOLCOH	Solubility of +V actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	8.75E-07	8.76E-07	7.39E-07	6.86E-07	6.60E-07	6.44E-07	moles/liter
	SOLSOH	Solubility of +V actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	3.90E-07	2.77E-07	2.18E-07	1.98E-07	1.88E-07	1.82E-07	moles/liter
SOLMOD6	SOLCOH	Solubility of +VI actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	moles/liter
	SOLSOH	Solubility of +VI actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	moles/liter

[(a)] Corresponds to $\left(S_{brine}^{red/ox}\right)$ in Equation 1.

Table 2. Actinide Solubility Uncertainty Parameters Used for the CRA-2009 PABC, and the CRA-2014 PA.

Material	Property	CRA-2009 PABC Value[(b)]	CRA-2009 PABC Value min and max[(d)]	CRA-2014 PA Value[(b)]	CRA-2014 PA Value min and max[(d)]	Units	Distribution Type
SOLMOD3	SOLVAR[(a)]	7.20E-02	-3.883, 2.439	-6.76E-01	-3.541, 2.643	NONE	Cumulative
SOLMOD4	SOLVAR[(a)]	-5.20E-01	-2.167, 3.244	6.60E-01	-1.156, 3.193	NONE	Cumulative
GLOBAL	OXSTAT[(c)]	5.00E-01	0.004, 0.995	5.00E-01	0.004, 0.995	NONE	Uniform

[(a)] Variability parameter for actinide solubility (*M* in Equation 2). SOLMOD3 is used for all actinides in the +III oxidation state and SOLMOD4 is used for the +IV oxidation state.
[(b)] Cumulative distributions for respective An(III) and An(IV) (Brush and Domski, 2013b) are used to define the solubility multiplier SOLVAR for the corresponding oxidation state III and IV model in the WIPP PA Parameter Database (PAPDB).
[(c)] If GLOBAL:OXSTAT is less than or equal to 0.5, Pu will be in oxidation state +III. If it is greater than 0.5, the oxidation state for plutonium will be +IV.
[(d)] Minimum and maximum values for the solubility multiplier SOLVAR used in the CRA-2014 PA and CRA-2009 PABC. These values come from **STP_CRA14_LHS_R1.TRN** in library **CRA14_STPW**, and **STP_PABC09_LHS_R1.TRN** in library **PABC09_STPW**.

2.2 SOLUBILITY UNCERTAINTY UPDATE

Brush and Domski (2013b) established the uncertainty range and probability distribution for the Th(IV) and Am(III) thermodynamic speciation and solubility models.

The Th(IV) comparison included a total of 185 measured and predicted Th(IV) solubilities, an increase of 45 from the 140 comparisons of Xiong et al. (2009) for the CRA-2009 PABC, in which ten general criteria (Xiong, Brush, Ismail and Long, 2009) were used for including results of experimentally measured solubilities in their comparisons of measured Th(IV), Nd(III), Am(III), and Cm(III) solubilities and predicted Th(IV) and Am(III) solubilities. The CRA-2014 PA used an additional criterion to include only results from experiment studies carried out under conditions at or close to those predicted for WIPP disposal rooms (Brush and Domski, 2013b). This additional criterion reduces a total of measured solubilities from 185 to 64. The WIPP Th(IV) model, the EQ3/6 code, and the DB **DATA0.FM1** over-predicted 14 of the 64 measured solubilities and under-predicted 50. The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Th(IV) solubilities are 0.673 and 1.029, respectively (see Table 5 in Brush and Domski, 2013b), and the mean and median values of the sampled uncertainty factor are $10^{0.673} = 4.708$ and $10^{1.029} = 10.703$. Xiong et al. (2009) used the same model, different database, and different code; and their mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Th(IV) solubilities were -0.346 and -0.520. See Xiong et al. (2009) for detailed descriptions of these results.

The Am(III) comparison included a total of 647 measured and predicted Nd(III) and Am(III) solubilities, an increase of 301 from the 346 comparisons of Xiong et al. (2009) for the CRA-2009 PABC. The above additional criterion reduces a total of measured solubilities from 647 to 172. The current comparison included more under-predictions than over-predictions. The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline

Am(III) solubilities are -0.678 and -0.866, respectively (Table 8 in Brush and Domski, 2013b), and the mean and median values of the sampled uncertainty factor are $10^{-0.678} = 0.210$ and $10^{-0.866} = 0.136$. Xiong et al. (2009) used the same model, different database, and different code; and their mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Am(III) solubilities were -0.142 and 0.072. See Xiong et al. (2009) for detailed descriptions of these results.

A thermodynamic speciation-and-solubility model has not been developed for U(VI) (Brush and Domski, 2013a). The EPA specified that a fixed value of 1×10^{-3} Moles/liter be used for U(VI). Beginning with the CRA-2004 PABC, the U(VI) solubility is fixed at 1×10^{-3} Moles/liter.

Actinide solubilities calculated by **EQ3/6** are modified by a variability factor (M) as shown in Equation 2:

$$\left(S_{brine}^{red/ox}\right) = \left(s_{brine}^{red/ox}\right) \cdot (10^{M}) \quad (2)$$

In this equation, $\left(S_{brine}^{red/ox}\right) = \left(s_{brine}^{red/ox}\right) \cdot (10^{M})$ is the solubility estimate for a given vector and M is a function of the oxidation state and is a sampled value as shown in Table 2.

2.3 INVENTORY UPDATE

The update to the CRA-2014 inventory was conducted by Los Alamos National Laboratory (LANL)(Van Soest, 2012). Calculation of the parameters needed for the CRA-2014 PA was conducted by SNL (Kicker and Zeitler, 2013). Table 3 shows the updated inventory values that are relevant for the PANEL calculations.

Table 3. Updated Radionuclide Inventory Values That Are Relevant to the PANEL Calculations for the CRA-2014 PA.

Material	Property	CRA-2009 PABC Value	CRA-2014 PA Value	Units
BOREHOLE	WUF[a]	2.60E+00	2.06E+00	Curies
AM241	INVCHD[b]	4.68E+05	6.97E+05	Curies
	INVRHD[c]	4.48E+03	8.06E+03	Curies
AM241L	INVCHD	4.85E+05	7.18E+05	Curies
	INVRHD	4.61E+03	8.56E+03	Curies
AM243	INVCHD	7.17E+01	2.18E+01	Curies
	INVRHD	7.80E-00	2.95E+01	Curies
CF252	INVCHD	3.28E-02	7.62E-01	Curies
	INVRHD	1.83E-04	9.26E-04	Curies
CM243	INVCHD	1.34E+00	2.16E+02	Curies
	INVRHD	2.09E+00	1.81E+01	Curies
CM244	INVCHD	2.63E+03	5.24E+03	Curies
	INVRHD	4.36E+02	4.73E+03	Curies
CM245	INVCHD	5.86E-01	3.70E-01	Curies
	INVRHD	8.26E-02	8.55E-01	Curies
CM248	INVCHD	1.24E-01	1.03E-01	Curies
	INVRHD	7.63E-03	1.62E-02	Curies
CS137	INVCHD	5.48E+02	2.31E+03	Curies
	INVRHD	8.89E+04	2.33E+05	Curies
NP237	INVCHD	3.65E+01	2.04E+01	Curies
	INVRHD	2.49E+00	2.84E+00	Curies
PA231	INVCHD	3.78E-01	5.88E-01	Curies
	INVRHD	1.87E-01	4.92E-02	Curies
PB210	INVCHD	1.75E+00	4.53E-01	Curies
	INVRHD	1.43E+01	1.38E+01	Curies
PM147	INVCHD	5.09E-02	1.00E-01	Curies
	INVRHD	1.18E+00	4.53E-01	Curies
PU238	INVCHD	1.47E+06	5.95E+05	Curies
	INVRHD	5.11E+03	5.80E+03	Curies
PU238L	INVCHD	1.47E+06	5.95E+05	Curies
	INVRHD	5.11E+03	5.80E+03	Curies
PU239	INVCHD	5.10E+05	5.67E+05	Curies
	INVRHD	2.92E+03	7.27E+03	Curies
PU239L	INVCHD	6.55E+05	7.60E+05	Curies
	INVRHD	3.92E+03	1.15E+05	Curies
PU240	INVCHD	1.44E+05	1.67E+05	Curies
	INVRHD	9.89E+02	7.94E+03	Curies
PU241	INVCHD	5.06E+05	6.48E+05	Curies
	INVRHD	3.94E+03	1.49E+04	Curies

Table 3. Updated Radionuclide Inventory Values That Are Relevant to the PANEL Calculations for the CRA-2014 PA (continued)

Material	Property	CRA-2009 PABC Value	CRA-2014 PA Value	Units
PU242	INVCHD	7.46E+01	1.66E+03	Curies
	INVRHD	1.25E+00	6.44E+03	Curies
PU244	INVCHD	3.48E-04	1.01E-02	Curies
	INVRHD	2.34E-06	7.38E-06	Curies
RA226	INVCHD	2.21E+00	6.19E-01	Curies
	INVRHD	1.83E+01	1.65E+01	Curies
RA228	INVCHD	3.08E-01	1.45E+00	Curies
	INVRHD	7.69E-02	1.76E-02	Curies
SR90	INVCHD	5.03E+02	2.31E+03	Curies
	INVRHD	7.99E+04	2.07E+05	Curies
TH229	INVCHD	8.81E+00	4.19E-01	Curies
	INVRHD	4.19E+00	9.81E-01	Curies
TH230	INVCHD	5.87E-01	4.13E+00	Curies
	INVRHD	9.20E-03	1.02E-02	Curies
TH230L	INVCHD	9.40E+00	4.54E+00	Curies
	INVRHD	4.20E+00	9.91E-01	Curies
TH232	INVCHD	2.75E-01	1.48E+00	Curies
	INVRHD	6.86E-02	1.46E-02	Curies
U233	INVCHD	1.56E+02	9.82E+01	Curies
	INVRHD	5.09E+01	4.04E+01	Curies
U234	INVCHD	3.04E+02	2.10E+02	Curies
	INVRHD	5.18E+00	3.23E+01	Curies
U234L	INVCHD	4.60E+02	3.08E+02	Curies
	INVRHD	5.61E+01	7.28E+01	Curies
U235	INVCHD	4.42E+00	8.66E+00	Curies
	INVRHD	7.04E-02	6.77E+01	Curies
U236	INVCHD	1.35E+00	5.08E+00	Curies
	INVRHD	2.48E-01	3.65E-01	Curies
U238	INVCHD	2.71E+01	3.51E+01	Curies
	INVRHD	2.96E-01	2.97E+01	Curies

(a) f_w in Equation 10.
(b) INVCHD is the inventory in contact-handled (CH) TRU waste.
(c) INVRHD is the inventory in remote-handled (RH) TRU waste.

2.4 PANEL IMPLEMENTATION

SNL originated the PANEL code for use in WIPP PA. PANEL version 3.60 was used in the CCA. Subsequently, PANEL was revised to Version 4.00 (Garner 1998) to simplify the PA calculation sequence, and to accommodate a change in the software that maintains the WIPP PAPDB. In preparation for the CRA-2004, PANEL was further revised to Version 4.02 to accommodate an increase in the number of sampled parameters for radionuclide solubilities (Garner 2003a). For the CRA-2004 PABC, PANEL was revised (Garner 2005a) to set the default volume of a panel via MATSET. PANEL 4.03 was validated according to the requirements of NP 19-1 (Garner 2003c) and used in the CRA-2004 PABC, CRA-2009 PA, CRA-2009 PABC and CRA-2014 PA calculations.

3. THEORETICAL BASIS FOR PANEL CALCULATIONS

WIPP PA deals with uncertainty in several ways. There is uncertainty in the appropriate value to assign to certain physical properties, like solubility, which is called subjective uncertainty. Subjective uncertainty is dealt with in WIPP PA (and in PANEL) by running multiple realizations in which the values of uncertain parameters are varied. For the WIPP PA, Latin Hypercube Sampling (LHS) (Vugrin 2005a) is used to create a "replicate" of 100 distinct parameter sets ("vectors") that span the full range of parameter uncertainty. To ensure that these LHS replicates are representative, a total of three replicates are run for a total of 300 separate vectors. Another type of uncertainty is what is called "stochastic" uncertainty, or the uncertainty in what will happen in the future. To deal with this type of uncertainty, WIPP PA employs a Monte Carlo method of sampling on random "futures". A future is defined as one possible sequence of events, or scenario. There are six scenarios defined for WIPP PA (Table 4). The total number of PANEL simulations that have to be run for a WIPP PA calculation is 300 vectors × 6 scenarios = 1800 PANEL model runs.

Table 4. WIPP PA modeling scenarios

Scenario	Description
S1	Undisturbed Repository
S2	E1 intrusion at 350 years
S3	E1 intrusion at 1000 years
S4	E2 intrusion at 350 years
S5	E2 intrusion at 1000 years
S6	E2 intrusion at 1000 years; E1 intrusion at 2000 years.

E1: Borehole penetrates through the repository and into a hypothetical pressurized brine reservoir in the Castile Formation.
E2: Borehole penetrates the repository, but does not encounter brine in the Castile. (Helton et al. 1998)

In WIPP PA scenarios, brine is assumed to enter the repository panels in either of two very different ways, namely: (a) by natural seepage from the surrounding Salado formation, and (b) by various locally-enhanced flows induced by hypothetical exploratory boreholes. In the case of the undisturbed scenario (S1), Salado brine can seep through the disturbed rock zone from the surrounding undisturbed halite and marker beds. In the case of a repository breached by an exploratory borehole (S2-S5), Castile and/or Culebra brine could flow into and through the repository via the pipe-like channels created by the borehole(s). An E1 intrusion assumes that a borehole passes through the repository and encounters a brine pocket in the Castile; an E2

intrusion is a borehole that does not encounter a brine pocket. The most intense flow (of Castile brine) would occur if a borehole that penetrates a waste panel also penetrates a deep pressurized brine pocket. The S6 scenario assumes that both an E1 and an E2 intrusion occur in the same waste panel. In this scenario, brine can flow from the Castile, through the waste in the panel, and then continue up an earlier, open borehole to the Culebra, (Helton et al. 1998).

PANEL's PA role is to estimate the mobilized radioactive contaminant load in the brine phase of the brine/gas mixture that seeps or flows through the repository's waste panels. Mobilization by any process, for example dissolution or suspension on colloids, is modeled as taking place instantaneously. The contaminants introduced into the brine are the aged radioisotopes that are assumed to reside in the repository at the time of closure plus any progeny of those radioisotopes that may have been produced through radioactive decay.

For WIPP PA, PANEL calculates: 1) decay and production over time for specified radionuclides, 2) concentrations of mobilized radionuclides, and 3) radionuclide quantities up the borehole to the Culebra for the S6 scenario. For each of these functions, an individual PANEL run is made. Thus, PANEL has three types of runs, the DECAY run type, the CONCENTRATION run type, and the STANDARD run type.

The following is a brief overview of the conceptual models implemented in PANEL for each of these run types. The conceptual models implemented in PANEL for the CRA-2014 PA are unchanged from those used in the CCA, the PAVT, the CRA-2004 PA, CRA-2004 PABC, CRA-2009 PA and CRA-2009 PABC.

3.1 RADIOACTIVE DECAY

The natural time scales associated with deep, tight-media, groundwater flows are typically centuries, and WIPP intrusion scenarios include temporal lapses of millennia prior to the hypothesized breaching of repository waste panels by boreholes. Moreover, EPA regulations extend to 10,000 years after decommissioning. On these time scales, radioisotopes of interest exhibit significant natural decay by which they transform to other radioactive and non-radioactive isotopes and/or compounds in a well-established way (Kaplan 1964). Thus, it is required to quantify the decay process and maintain a running record of the decayed contents of the repository as well as all the products of decay from the time of closure onward to 10,000 years.

This is performed in PANEL for all three run types: DECAY, CONCENTRATION, or STANDARD. If the user wishes to obtain an output file with the decayed values, the DECAY run type has to be used. The DECAY run type decays the radionuclide inventory for 10,000 years and outputs the results.

The equations that quantify the decay-and-growth cycle of isotopes were first described by Bateman (1910) and traditionally bear his name. Bateman's equations state that the rate at which the mass of a radioisotope decreases by natural radioactive decay is proportional to the present available mass of that radioisotope. In single decays, the constant of proportionality is the natural logarithm of 2 divided by the half-life of the isotope in question. If the isotope in question is other than the first isotope in the chain, its mass will also increase at a rate

proportional to the present mass of its parent isotope. In simple decay chains, the constant of proportionality is the natural logarithm of 2 divided by the half-life of the parent. In multiple (i.e., bifurcated) chains, the decay algebra is slightly more complicated. However, the simple decay chains used in WIPP PAs have no bifurcations. The formulation and solution for Bateman's equations in PANEL are given in Section 4.4 of the PANEL User's Manual (Garner 2003b).

PANEL solves the Bateman equations at each time step (50 year time steps). In addition to the radionuclide inventory that is an input for this calculation (shown in Table 3), PANEL needs the atomic weight and half-life of the radionuclides. These values are shown in Table 5 and have not changed since the CCA. In the DECAY mode, PANEL decays those radionuclides shown in Table 5.

Table 5. Atomic Weights and Radionuclide Half-lives for CRA-2014 PA

Material	Property	CRA-2014 PA Value	Units	Material	Property	CRA-2014 PA Value	Units
AM241	ATWEIGHT	2.41E-01	kg/mole	PU241	ATWEIGHT	2.41E-01	kg/mole
	HALFLIFE	1.36E+10	s		HALFLIFE	4.54E+08	s
AM243	ATWEIGHT	2.43E-01	kg/mole	PU242	ATWEIGHT	2.42E-01	kg/mole
	HALFLIFE	2.33E+11	s		HALFLIFE	1.22E+13	s
CF252	ATWEIGHT	2.52E-01	kg/mole	PU244	ATWEIGHT	2.44E-01	kg/mole
	HALFLIFE	8.33E+07	s		HALFLIFE	2.61E+15	s
CM243	ATWEIGHT	2.43E-01	kg/mole	RA226	ATWEIGHT	2.26E-01	kg/mole
	HALFLIFE	8.99E+08	s		HALFLIFE	5.05E+10	s
CM244	ATWEIGHT	2.44E-01	kg/mole	RA228	ATWEIGHT	2.28E-01	kg/mole
	HALFLIFE	5.72E+08	s		HALFLIFE	2.11E+08	s
CM245	ATWEIGHT	2.45E-01	kg/mole	SR90	ATWEIGHT	8.99E-02	kg/mole
	HALFLIFE	2.68E+11	s		HALFLIFE	9.19E+08	s
CM248	ATWEIGHT	2.48E-01	kg/mole	TH229	ATWEIGHT	2.29E-01	kg/mole
	HALFLIFE	1.07E+13	s		HALFLIFE	2.32E+11	s
CS137	ATWEIGHT	1.37E-01	kg/mole	TH230	ATWEIGHT	2.30E-01	kg/mole
	HALFLIFE	9.47E+08	s		HALFLIFE	2.43E+12	s
NP237	ATWEIGHT	2.37E-01	kg/mole	TH232	ATWEIGHT	2.32E-01	kg/mole
	HALFLIFE	6.75E+13	s		HALFLIFE	4.43E+17	s
PA231	ATWEIGHT	2.31E-01	kg/mole	U233	ATWEIGHT	2.33E-01	kg/mole
	HALFLIFE	1.03E+12	s		HALFLIFE	5.00E+12	s
PB210	ATWEIGHT	2.10E-01	kg/mole	U234	ATWEIGHT	2.34E-01	kg/mole
	HALFLIFE	7.04E+08	s		HALFLIFE	7.72E+12	s
PM147	ATWEIGHT	1.47E-01	kg/mole	U235	ATWEIGHT	2.35E-01	kg/mole
	HALFLIFE	8.28E+07	s		HALFLIFE	2.22E+16	s
PU238	ATWEIGHT	2.38E-01	kg/mole	U236	ATWEIGHT	2.36E-01	kg/mole
	HALFLIFE	2.77E+09	s		HALFLIFE	7.39E+14	s
PU239	ATWEIGHT	2.39E-01	kg/mole	U238	ATWEIGHT	2.38E-01	kg/mole
	HALFLIFE	7.59E+11	s		HALFLIFE	1.41E+17	s
PU240	ATWEIGHT	2.40E-01	kg/mole				
	HALFLIFE	2.06E+11	s				

3.2 POTENTIAL FOR DISSOLUTION AND MOBILIZATION

PANEL calculates what is in essence the potential for dissolution and mobilization of an actinide in a brine. It is called a potential here because it is basically the limit on how much material can be dissolved and/or mobilized in a brine if the inventory of the material is unlimited. This potential would be equal to the solubility in the absence of colloids. In the presence of colloids, the potential includes dissolved species and mobilized colloidal species. Like solubility, the units for the mobilization potential is moles/liter.

The dissolved component of the mobilization potential is calculated using Equation 2 from Section 2.2. The base solubility value, $(s_{brine}^{red/ox})$, is one of the values from Table 1, depending on the oxidation state of the actinide and the brine type for the vector. Since microbial activity is present for all vectors in the CRA-2004 PABC, CRA-2009 PABC and CRA-2014 PA, the carbon dioxide (CO_2) would be produced by consuming all of the cellulosic, plastic, and rubber (CPR) materials in the repository. MgO, as is used in the WIPP, will decrease actinide solubilities by consuming CO_2 (U.S. DOE, 2009). The variable, *M*, is sampled from one of the distributions shown in Table 2 depending on the oxidation state of the actinide.

Once the dissolution potential is known, the colloidal mobilization potentials are determined by means of proportionality factors or by constants. The mobilization potential for humic colloids is calculated using Equation 3 (U.S. DOE 2004 Appendix SOTERM).

$$H_{brine}^{red/ox} = \begin{cases} \left(S_{brine}^{red/ox}\right) \bullet \left(h_{brine}^{red/ox}\right) & if \left(S_{brine}^{red/ox}\right) \bullet \left(h_{brine}^{red/ox}\right) \le \left(H_{elem}^{\max}\right) \\ \left(H_{elem}^{\max}\right) & if \left(S_{brine}^{red/ox}\right) \bullet \left(h_{brine}^{red/ox}\right) > \left(H_{elem}^{\max}\right) \end{cases} \quad (3)$$

$H_{brine}^{red/ox}$ is the mobilization potential for humic colloids. $(S_{brine}^{red/ox})$ is defined in Equation 2. $\left(h_{brine}^{red/ox}\right)$ is a factor for humic colloids that is defined for each oxidation state and brine type as shown in Table 6. $\left(H_{elem}^{\max}\right)$ is the maximum allowed for mobilized humic colloids for the element (also shown in Table 6). None of the values in Table 6 were updated for the CRA-2014 PA.

The mobilization potential for mineral fragment colloids is as shown in Equation 4.

$$MF_{brine}^{red/ox} = \left(mf_{brine}^{red/ox}\right) \quad (4)$$

$MF_{brine}^{red/ox}$ is the mobilization potential for mineral fragment colloids. $\left(mf_{brine}^{red/ox}\right)$ is a constant value for each element that is independent of brine type as shown in Table 7. None of the values in Table 7 were updated for the CRA-2014 PA.

The mobilization potential for intrinsic colloids is as shown in Equation 5.

$$IC_{brine}^{red/ox} = \left(ic_{brine}^{red/ox}\right) \quad (5)$$

$IC_{brine}^{red/ox}$ is the mobilization potential for intrinsic colloids. $\left(ic_{brine}^{red/ox}\right)$ is a constant value for each element that is independent of brine of type as shown in Table 8. The values in Table 8 were updated for the CRA-2014 PA.

The mobilization potential for microbial colloids is zero if there is no microbial activity. However all vectors have microbial activity in the CRA-2014 PA. The mobilization potential for microbial colloids is calculated using Equation 6.

Table 6. Parameters related to humic colloids for the CRA-2014 PA

Material	Property	Description	CRA-2014 PA Value	Units
PHUMOX3	PHUMCIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +III oxidation state in Castile brine	[a]1.37E+00	NONE
	PHUMSIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +III oxidation state in Salado brine	1.90E-01	NONE
PHUMOX4	PHUMCIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +IV oxidation state in Castile brine	6.30E+00	NONE
	PHUMSIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +IV oxidation state in Salado brine	6.30E+00	NONE
PHUMOX5	PHUMCIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +V oxidation state in Castile brine	7.40E-03	NONE
	PHUMSIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +V oxidation state in Salado brine	9.10E-04	NONE
PHUMOX6	PHUMCIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +VI oxidation state in Castile brine	5.10E-01	NONE
	PHUMSIM[b]	Multiplicative factor to calculate humic colloids for actinides in the +VI oxidation state in Salado brine	1.20E-01	NONE
AM	CAPHUM[C]	Maximum concentration for humic colloids for Am	1.10E-05	moles/liter
NP	CAPHUM[C]	Maximum concentration for humic colloids for Np	1.10E-05	moles/liter
PU	CAPHUM[C]	Maximum concentration for humic colloids for Pu	1.10E-05	moles/liter
TH	CAPHUM[C]	Maximum concentration for humic colloids for Th	1.10E-05	moles/liter
U	CAPHUM[C]	Maximum concentration for humic colloids for U	1.10E-05	moles/liter

[a] This is a median value of a cumulative distribution (Tierney, 1996).

[b] Corresponds to $\left(h_{brine}^{red/ox}\right)$ in Equation 3.

[c] Corresponds to $\left(H_{elem}^{\max}\right)$ in Equation 3.

Table 7. Parameters related to mineral fragment colloids for the CRA-2014 PA

Material	Property	Description	CRA-2014 PA Value	Units
AM	CONCMIN[(a)]	Concentration for mineral colloids for Am	2.60E-08	moles/liter
NP	CONCMIN	Concentration for mineral colloids for Np	2.60E-08	moles/liter
PU	CONCMIN	Concentration for mineral colloids for Pu	2.60E-08	moles/liter
TH	CONCMIN	Concentration for mineral colloids for Th	2.60E-08	moles/liter
U	CONCMIN	Concentration for mineral colloids for U	2.60E-08	moles/liter

(a) Corresponds to $\left(mf_{brine}^{red/ox}\right)$ in Equation 4.

Table 8. Parameters related to intrinsic colloids for the CRA-2014 PA

Material	Property	Description	CRA-2014 PA Value	Units
AM	CONCINT[(a)]	Concentration for intrinsic colloids for Am	4.00E-09	moles/liter
NP	CONCINT	Concentration for intrinsic colloids for Np	2.00E-08	moles/liter
PU	CONCINT	Concentration for intrinsic colloids for Pu	2.00E-08	moles/liter
TH	CONCINT	Concentration for intrinsic colloids for Th	2.00E-08	moles/liter
U	CONCINT	Concentration for intrinsic colloids for U	3.00E-08	moles/liter

(a) Corresponds to $\left(ic_{brine}^{red/ox}\right)$ in Equation 5.

Table 9. Parameters related to microbial colloids for the CRA-2014 PA

Material	Property	Description	CRA-2014 PA Value	Units
AM	PROPMIC[(a)]	Multiplicative factor to calculate microbial colloids for Am	3.20E-01	NONE
NP	PROPMIC	Multiplicative factor to calculate microbial colloids for Np	1.76E+00	NONE
PU	PROPMIC	Multiplicative factor to calculate microbial colloids for Pu	1.76E+00	NONE
TH	PROPMIC	Multiplicative factor to calculate microbial colloids for Th	1.76E+00	NONE
U	PROPMIC	Multiplicative factor to calculate microbial colloids for U	1.76E+00	NONE
AM	CAPMIC[(b)]	Maximum concentration for microbial colloids for Am	3.10E-08	moles/liter
NP	CAPMIC	Maximum concentration for microbial colloids for Np	2.30E-06	moles/liter
PU	CAPMIC	Maximum concentration for microbial colloids for Pu	2.30E-06	moles/liter
TH	CAPMIC	Maximum concentration for microbial colloids for Th	2.30E-06	moles/liter
U	CAPMIC	Maximum concentration for microbial colloids for U	2.30E-06	moles/liter

(a) Corresponds to $\left(mc_{brine}^{red/ox}\right)$ in Equation 6.

(b) Corresponds to $\left(MC_{elem}^{\max}\right)$ in Equation 6.

$$MC_{brine}^{red/ox} = \begin{cases} \left(S_{brine}^{red/ox}\right)\bullet\left(mc_{brine}^{red/ox}\right) & if \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right)+\left(S_{brine}^{red/ox}\right)\bullet\left(mc_{brine}^{red/ox}\right) < \left(MC_{elem}^{\max}\right) \\ 0 & if \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right) > \left(MC_{elem}^{\max}\right) \\ \left(MC_{elem}^{\max}\right)-\left(S_{brine}^{red/ox}\right)-\left(H_{brine}^{red/ox}\right)-\left(MF_{brine}^{red/ox}\right)-\left(IC_{brine}^{red/ox}\right) & \end{cases} \quad (6)$$

$$if \begin{cases} \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right) < \left(MC_{elem}^{\max}\right) \\ and \\ \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right)+\left(S_{brine}^{red/ox}\right)\bullet\left(mc_{brine}^{red/ox}\right) > \left(MC_{elem}^{\max}\right) \end{cases}$$

$MC_{brine}^{red/ox}$ is the mobilization potential for microbial colloids. $\left(S_{brine}^{red/ox}\right)$ is defined in Equation 2. $\left(H_{brine}^{red/ox}\right)$ is defined in Equation 3. $\left(MF_{brine}^{red/ox}\right)$ is defined in Equation 4. $\left(IC_{brine}^{red/ox}\right)$ is defined in Equation 5. $\left(mc_{brine}^{red/ox}\right)$ is a multiplicative factor for microbial colloids that is defined for each element independent of brine type as shown in Table 9. $\left(MC_{elem}^{\max}\right)$ is a value that limits the amount of microbial colloids that can be mobilized in the presence of other mobilization processes. The values for $\left(MC_{elem}^{\max}\right)$ are shown in Table 9. All the values in Table 9 were updated for the CRA-2014 PA.

The total mobilization potential is the sum of the dissolution potential and the mobilization potentials for the four colloids as shown in Equation 7.

$$TC_{brine}^{red/ox} = \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MC_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right) \quad (7)$$

$TC_{brine}^{red/ox}$ is the total mobilization potential.

3.3 MOBILIZED RADIONUCLIDE CONCENTRATIONS

PANEL computes the concentration of radionuclides mobilized in a panel that contains a given volume of brine. This is performed in PANEL using the CONCENTRATION run type. The total mobilized concentration consists of a dissolved component and up to four colloidal components: humic, microbial, intrinsic, and mineral fragment colloids.

The dissolution part of PANEL's waste-mobilization-and-transport model is based on the following assumptions: (1) The concentration of each brine-dissolved element is uniform (i.e., constant) throughout a waste panel. (2) Mobilization is assumed to take place instantaneously and to maximum capacity, i.e., to saturation if inventory permits. (3) Supersaturation is disallowed. (4) When an element has several isotopes, the molar proportions of those isotopes dissolved in the brine are taken to be the same as the molar proportions in the total inventory contained in the waste panel, and (5) the fraction of the inventory in the panel is 0.105148 (updated for CRA-2014 PA). The value 0.105148 is the ratio of the area of one panel to the area of all ten panels. For CRA-2014 PA, the fraction of the inventory is calculated in an ALGEBRA step before PANEL is executed (Clayton, 2009a)

The concentration is given in Equation 8.

$$C_{brine}^{isotope} = \min\left\{\frac{\sum_i N^{isotope}}{V_{brine}}, TC_{brine}^{red/ox}\right\} \bullet \left\{\frac{N^{isotope}}{\sum_i N^{isotope}}\right\} \quad (8)$$

Where $C_{brine}^{isotope}$ is the concentration in moles/liter for the isotope. $N^{isotope}$ is the total moles of the isotope in the inventory, $\sum_i N^{isotope}$ is the sum of all isotopes of the element that contains the isotope of interest, and V_{brine} is the volume of brine in contact with the inventory. For the mobilized radionuclide concentration calculations, the brine volume, V_{brine}, is a constant value based on Stein (2005) for the CRA-2004 PABC, Clayton (2008) for the CRA-2009 PABC and Camphouse (2013) for the CRA-2014 PA. The value derived in Stein (2005), Clayton (2008) or Camphouse (2013) is the minimum volume of brine required for a Direct Brine Release (DBR). The minimum volume is used because it leads to the highest value for $C_{brine}^{isotope}$. Converting to activity,

$$a_{brine}^{isotope} = C_{brine}^{isotope} \bullet MW^{isotope} \bullet SP^{isotope} \quad (9)$$

Where $a_{brine}^{isotope}$ is the activity concentration in Ci/liter for the isotope. $C_{brine}^{isotope}$ is defined in Equation 8. $MW^{isotope}$ is the molecular weight of the isotope in g/mole, and $SP^{isotope}$ is the specific activity of the isotope in Ci/g.

The EPA units are defined using Equation 10.

$$W^{isotope} = \frac{\left(a_{brine}^{isotope}\right)}{L_{isotope} \bullet f_w} \quad (10)$$

where $W^{isotope}$ is the activity concentration in EPA Units/liter for the isotope. $L_{isotope}$ is the EPA release limit for the isotope (shown in Table 10), and f_w is the waste unit factor (shown in Table 3, defined in Leigh and Trone 2005b). None of the values in Table 10 were updated for the CRA-2014 PA.

Table 10. Parameters related to calculation of total mobilized EPA units in PANEL.

Material	Property	CRA-2004 PABC Value	CRA-2009 PABC Value	CRA-2014 PA Value	Units
AM241	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
AM243	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
CF252	EPAREL	0.00E+00	0.00E+00	0.00E+00	Curies/wuf
CM243	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
CM244	EPAREL	0.00E+00	0.00E+00	0.00E+00	Curies/wuf
CM245	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
CM248	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
CS137	EPAREL	1.00E+03	1.00E+03	1.00E+03	Curies/wuf
NP237	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PA231	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PB210	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PM147	EPAREL	0.00E+00	0.00E+00	0.00E+00	Curies/wuf
PU238	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PU239	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PU240	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PU241	EPAREL	0.00E+00	0.00E+00	0.00E+00	Curies/wuf
PU242	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
PU244	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
RA226	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
RA228	EPAREL	0.00E+00	0.00E+00	0.00E+00	Curies/wuf
SR90	EPAREL	1.00E+03	1.00E+03	1.00E+03	Curies/wuf
TH229	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
TH230	EPAREL	1.00E+01	1.00E+01	1.00E+01	Curies/wuf
TH232	EPAREL	1.00E+01	1.00E+01	1.00E+01	Curies/wuf
U233	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
U234	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
U235	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
U236	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf
U238	EPAREL	1.00E+02	1.00E+02	1.00E+02	Curies/wuf

PANEL solves Equations 8 through 10 at each time step (50 year time steps). The formulation and solution for Equations 8 through 10 in PANEL are given in Section 4.3 of the PANEL User's Manual (Garner 2003b). Mobilized radionuclide concentrations are calculated for the 23 individual radionuclides and five "lumped" radionuclides shown in Table 11. The "lumped" radionuclides are defined as (Leigh and Trone 2005a):

AM241L is the amount of AM241 plus the amount of PU241.
PU238L is the same amount as PU238.
PU239L is the amount of PU239 plus the amount of PU240 plus the amount of PU242.
U234L is the amount of U234 plus the amount of U233.
TH230L is the amount of TH230 plus the amount of TH229.

"Lumped" radionuclides are used to ease the burden associated with calculation of radionuclide transport in some of the WIPP PA codes: NUTS (Leigh 2003) which calculates Salado transport and CCDFGF (Vugrin 2004) which calculates Culebra releases.

Table 11: Radionuclides Modeled in PANEL Concentration Calculations

Individual Radionuclides				
AM241	CM248	PU238	**RA226**	U233
AM243	CS137	PU239	**RA228**	U234
CF252[(a)]	NP237	PU240	SR90	U235
CM243	**PA231**	PU241	TH229	U236
CM244	**PB210**	PU242	TH230	U238
CM245	PM147	PU244	TH232	
Lumped Radionuclides				
AM241L	PU238L	PU239L	TH230L	U234L

[(a)] The isotopes shown in bold are included in the decay calculations but are not included in the mobilization calculations.

PANEL supplies information from the CONCENTRATION run to NUTS and CCDFGF. For NUTS the values supplied by PANEL are defined in Equation 11.

$$\left\{TC_{brine}^{red/ox}\right\}_{NUTS} = TC_{brine}^{red/ox} \bullet 10^{-L_{dif}^{sol}} \tag{11}$$

Where $\left\{TC_{brine}^{red/ox}\right\}_{NUTS}$ is the potential moles per liter mobilized for the lumped isotopes in Table 11. L_{dif}^{sol} is a multiplicative factor used to account for molar proportions of isotopes in the inventory. The multiplicative factors are calculated in two ALGEBRACDB steps and set in the parameters, PU238L:LSOLDIF, TH230L:LSOLDIF, U234L:LSOLDIF. Calculation of these values is discussed in Clayton, 2009a and Appendix A.

The total concentration in EPA units for the 23 individual radionuclides is used by CCDFGF to calculate DBR. For the calculation of DBR in CCDFGF, the values supplied by PANEL are defined in Equation 12.

$$W^{total} = \sum_{isotopes} W^{isotope} \quad (12)$$

W^{total} is the total EPA units per liter for the 23 individual isotopes in Table 11. For the calculation of Culebra releases (S1-S5) in CCDFGF, the values supplied by PANEL are defined by Equation 13.

$$W^{total}_{lumped} = \sum_{lumped} W^{isotope} \quad (13)$$

W^{total}_{lumped} is the total EPA Units per liter for the lumped isotopes in Table 11.

3.4 RADIONUCLIDES UP THE BOREHOLE TO THE CULEBRA (S6)

PANEL also computes the quantities of "lumped" radionuclides that move up the borehole to the Culebra for the S6 scenario. This is performed in PANEL using the STANDARD run type.

The PANEL calculation for S6 is similar to that discussed in Section 3.3 except that the panel brine volume and the brine flow volumes are supplied by BRAGFLO (Nemer 2006). PANEL conservatively assumes that any radionuclide that rises above the disturbed rock zone above the waste panels reaches the Culebra. The formulation and solution for this calculation in PANEL are given in Section 4.5 of the PANEL User's Manual (Garner 2003b).

4. PANEL MODELING PROCESS

Digital Command Language (DCL) scripts, referred to here as EVAL run scripts, are used to implement and document the running of all software codes for the WIPP PA. These scripts, which are the basis for the WIPP PA run control system, are stored in the CRA14_EVAL Configuration Management System (CMS) library. All inputs are fetched at run time by the scripts, and outputs and run logs are automatically stored by the scripts in class CRA14-0 of the CMS libraries (Long, 2013).

Figure 1 (left hand side) shows the run sequence for PANEL. For the CRA-2014 PA, PANEL was run in the DECAY mode to produce decayed radionuclide inventories. This run is independent of scenario and only needs to be run once. Two ALGEBRACDB runs follow the DECAY run to set parameters for the following PANEL runs.

PANEL was also run in the CONCENTRATION mode for Scenarios S1 through S5. This is represented on the left-hand-side of Figure 1 where GENMESH (Stein 2003c) provides input to MATSET (Gilkey 2003b). MATSET provides input to POSTLHS (Vugrin 2005b), and POSTLHS provides input to ALGEBRACDB (Gilkey 2003a). Output from this third ALGEBRACDB run is input to PANEL.

PANEL was also run in the STANDARD mode for Scenario S6. This is represented by the entirety of Figure 1 where the output from ALGEBRACDB on the left-hand-side of the figure is

input to PANEL and the output from POSTBRAG (Stein 2003b) and ALGEBRACDB is also input to PANEL. The software version numbers used for the PANEL calculations for the CRA-2014 PA are given in Table 12.

Table 12. Software Version Numbers Used for PANEL Calculations for the CRA-2014 PA

Software Application	Version
GENMESH	6.08
MATSET	9.20
POSTLHS	4.07A
ALGEBRACDB	2.35
SUMMARIZE	3.01
STEPWISE	2.21
PCCSRC	2.21

4.1 GENMESH: SINGLE-ELEMENT GRID GENERATION

The first step in the PANEL modeling process is the definition of a single-element grid (one block) using the GENMESH code (Stein 2003c). The analyst supplies input for GENMESH in an ASCII input file. The CRA-2014 PA analysis uses the file: **GM_PANEL_CRA14.INP** (see Appendix B) located in CMS library: **CRA14_PANEL**.

4.2 MATSET: MATERIAL PROPERTY ASSIGNMENTS

Details of the functionality of MATSET are discussed in the users manual (Gilkey 2003b). MATSET assigns the material property values needed by PANEL. The GENMESH binary output file (**GM_PANEL_CRA14.CDB**), which is required as input for the MATSET code, provides the initial material map. All materials and properties that are used in PANEL modeling should be specified in this modeling step, although the values may be changed in subsequent steps. For example, the parameters that are assigned sampled values by the LHS code (Vugrin 2005a), must be assigned initial values by MATSET in order that they can be reassigned in later steps.

Each property assignment requires specification of both the material (e.g. Pu) and the property (e.g. maximum concentration for microbial colloids for Pu) to be associated with that material. For PA analyses, MATSET extracts the information from the WIPP PAPDB according to instructions in the user-supplied input control file. If the database contains information defining a distribution of values for a material/property pair, MATSET retrieves the median value. The MATSET input file used for the CRA-2014 PA is **MS_PANEL_CRA14.INP** (see Appendix B) and is located in the CMS library: **CRA14_PANEL**.

Like the CRA-2009 PABC calculation procedure, three additional steps were proceeded before the POSTLHS step. PANEL was executed in the decay mode and then ALGEBRA was run twice. These steps were done in order that the mole fractions for the lumped variables and the fraction of inventory in one panel could be calculated as part of the run stream instead of being done offline (Clayton, 2009b).

4.3 POSTLHS: UNCERTAIN PARAMETER VALUES

The sixth step in the run sequence employs the POSTLHS code, which takes the binary output from the second algebra step (**ALG2_PANEL_CRA14BV*k*.09.CDB**, k = 1, 2, 3, 4, 5) and creates 100 copies of this file replacing median values with the sampled values for every sampled parameter in each vector. The sampled parameters for PANEL are: GLOBAL:OXSTAT, PHUMOX3:PHUMCIM, SOLMOD3:SOLVAR, SOLMOD4:SOLVAR, and WAS_AREA:PROBDEG. The sampled parameter WAS_AREA:PROBDEG no longer has any impact on the source term since the distribution has been changed, so there is always microbial degradation. POSTLHS requires that a dummy ASCII file be specified, which is not used in the calculations. The dummy file used for the CRA-2014 PA is **LHS3_DUMMY.INP** (see Appendix B) and is located in CMS library: **LIBCRA14_LHS**. Output from LHS (**LHS2_PANEL_CRA14_R1.TRN**, **LHS2_PANEL_CRA14_R2.TRN**, **LHS2_PANEL_CRA14_R3.TRN** for the three replicates) are also used by POSTLHS in this step. These files are stored in CMS library: **CRA14_LHS**.

4.4 ALGEBRACDB: DATA MODIFICATION

The next modeling step employs the ALGEBRACDB code which is used to manipulate data from the binary output files from POSTLHS. ALGEBRACDB is capable of performing most common algebraic manipulations and evaluating most common transcendental functions (trigonometric, logarithmic, exponential, etc.). Its functionality is discussed in the users manual (Gilkey 2003a).

ALGEBRACDB reads its instructions from a user-supplied ASCII input file that employs an algebraic syntax that is similar in appearance to FORTRAN syntax. The ALGEBRACDB input file used for this step in the CRA-2014 PA is **ALG3_PANEL_CRA14BV*k*.INP** (k = 1, 2, 3, 4 or 5) (see Appendix B) and is located in CMS library: **LIBCRA14_PANEL**. It executes the mathematical instructions to modify the output data from POSTLHS:

- **LHS3_PANEL_CRA14BV*k*_R1_V001.CDB - LHS3_PANEL_CRA14BV*k*_R1_V100.CDB;**
- **LHS3_PANEL_CRA14BV*k*_R2_V001.CDB - LHS3_PANEL_CRA14BV*k*_R2_V100.CDB;**

and

- **LHS3_PANEL_CRA14BV*k*_R3_V001.CDB - LHS3_PANEL_CRA14BV*k*_R3_V100.CDB**

which are stored in the CMS library: **CRA14_PANEL**.

The results are written to new binary (.CDB) output files:

- **ALG3_PANEL_CRA14BV*k*_R1_V001.CDB – ALG3_PANEL_CRA14BV*k*_R1_V100.CDB;**
- **ALG3_PANEL_CRA14BV*k*_R2_V001.CDB – ALG3_PANEL_CRA14BV*k*_R2_V100.CDB;**

and

- **ALG3_PANEL_CRA14BV*k*_R3_V001.CDB – ALG3_PANEL_CRA14BV*k*_R3_V100.CDB**

Which are stored in the CMS library: **CRA14_PANEL**.

4.5 BRAGFLO OUTPUT TO PANEL

As mentioned above, for the S6 scenario, PANEL requires BRAGFLO results (right-hand-side of Figure 1). The required PANEL input for the S6 scenario is generated by the BRAGFLO run and is stored in the files **ALG2_BF_CRA14_R1_S6_V001.CDB** through **ALG2_BF_CRA14_R3_S6_V100.CDB** which are stored in the CMS libraries **CRA14_BFR*x*S6**, where *x*=1, 2, or 3.

4.6 SUMMARIZE

Panel files are stored in CMS library **CRA14_PANEL** and are named **PANEL_INT_CRA14BV*k*_R*r*_S6_TI*tttt*_V001.CDB** through **PANEL_INT_CRA14BV*k*_R*r*_S6_TI*tttt*_V100.CDB**, where r = 1, 2, 3, and *tttt* = 0100, 0350, 1000, 2000, 4000, 6000, 9000 for the S6 type runs.

Panel decay runs are named **PANEL_DECAY_CRA14_R1_S1_V001.CDB** and Panel concentration runs are named **PANEL_CON_CRA14BV*k*_R*r*_S*s*_V001.CDB** to **PANEL_CON_CRA14BV*k*_R*r*_S*s*_V100.CDB**, where s = 1, 2, 3, 4, 5.

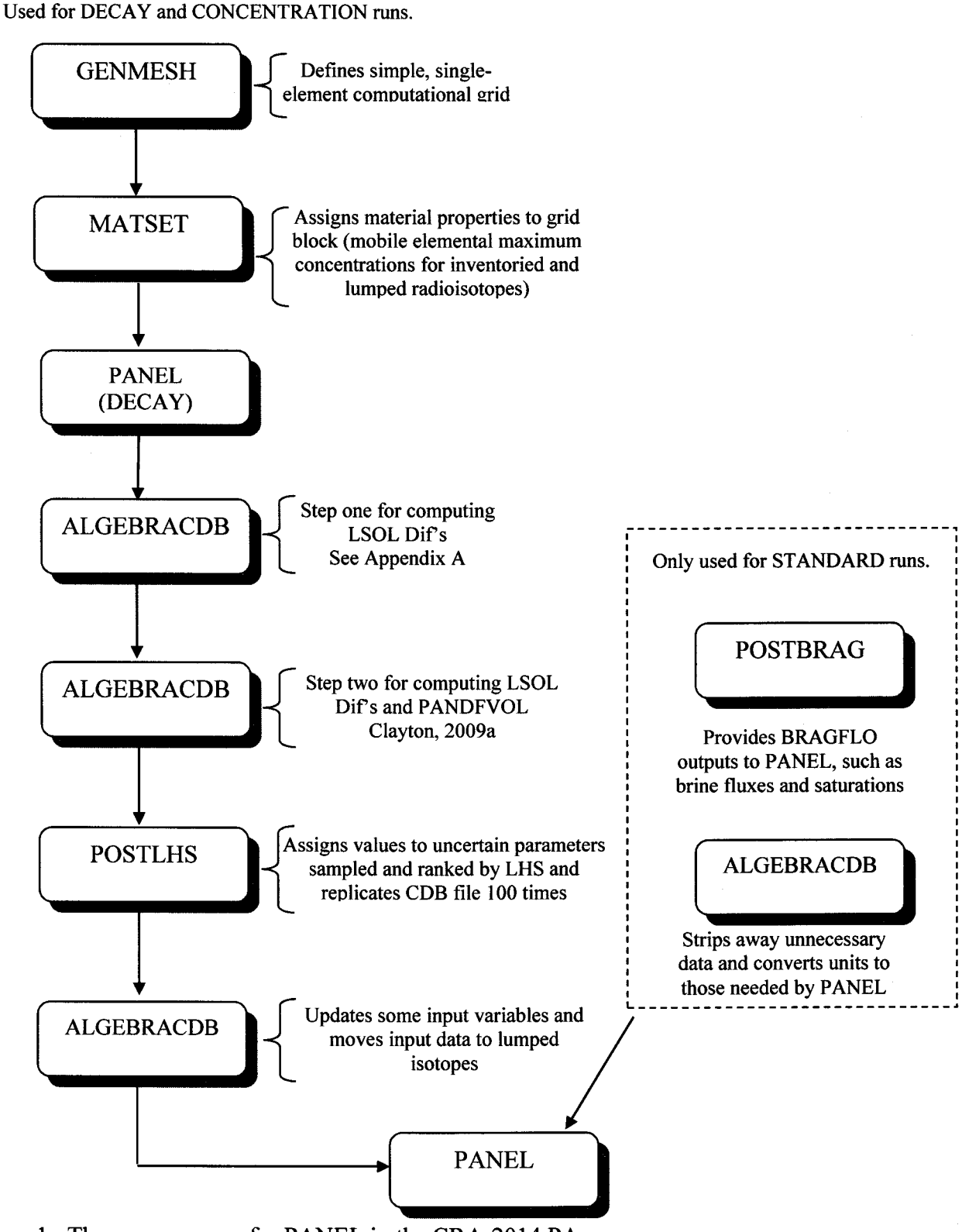


Figure 1. The run sequence for PANEL in the CRA-2014 PA.

5. PANEL RESULTS

PANEL is unique in the performance assessment framework in that it produces information for several of the downstream WIPP PA codes: NUTS (for Salado transport), CCDFGF (for Culebra releases), and CCDFGF (for DBR releases). The calculated outputs in each case are different. In addition, PANEL is frequently used in a stand-alone mode to calculate radionuclide decay.

NUTS needs information for the "lumped" radionuclides AM241L, PU238L, PU239L, U234L, and TH230L. CCDFGF (for DBR releases) needs the mobilized radionuclide concentrations in brine (Salado and/or Castile brine) reported as the sum of the EPA units for the 23 isotopes listed in Table 11 (the non-bold isotopes in Table 11). CCDFGF (for Culebra releases in the S6 scenario) needs the EPA units of the "lumped" radionuclides AM241L, PU238L, PU239L, U234L, and TH230L up the borehole to the Culebra.

PANEL is run in the CONCENTRATION mode for Scenarios S1, S2, S3, S4, and S5. The concentrations for S1, S4, and S5 are all equivalent (as they all involve Salado brine), as are the concentrations for S2 and S3 (Castile brine). The concentration data for S1 (Salado brine) and S2 (Castile brine) are used together with DBR volumes to obtain radionuclide releases through the DBR pathway in CCDFGF. PANEL is run in the STANDARD mode for S6.

Calculation of the mobilized concentration is a three step process that starts with calculation of the potential for a particular brine to contain both dissolved and mobilized colloidal components of an element. If colloidal components were not involved (an element with only a dissolved component), this potential would be the solubility of the element in the brine. When colloidal components are involved, the potential has been referred to in previous PANEL documents as the "source term" for an element. The "source term" corresponds to the moles of an element that can be mobilized in a liter of brine (either through dissolution and/or colloidal suspension) if the inventory of the element is unlimited. It loosely corresponds to what is known in other chemical applications as the saturation state.

Once the potential that a particular brine has to contain dissolved and mobilized colloidal components of an element has been established, then the inventory of the element that is available for mobilization is required. If there is more material available for mobilization than the brine can hold, the concentration in the brine will be equivalent to "saturation." If there is less material available for mobilization than the brine can hold, the concentration in the brine will be equivalent to the inventory value divided by the brine volume.

The inventory value is a function of time because of radioactive decay and production. Isotopes (of which an element is comprised) decay and produce other isotopes as discussed in Section 3.1. At any given time, the isotopic mix in the inventory and thus the elemental mix in the inventory will change. Plus, material can be removed from the panel. Thus, the second step in the calculation of mobilized concentrations is determining the remaining inventory as a function of time.

Once the available inventory is determined, the volume of brine in contact with the inventory is required. PANEL computes mobilized radionuclide concentrations in a panel that contains a given volume of brine. The volume of brine for the CONCENTRATION run is an assumed

quantity based on Camphouse (2013) for the CRA-2014 PA. Camphouse (2008) gives estimates of the brine volume in the repository that would lead to a brine release. These values are 1 ×, 2 ×, 3 ×, 4 × and 5 × 17,400 m^3. To determine the fraction of these volumes that would be in a panel, the volume value is multiplied by the fraction of one panel to the entire repository. The volume of brine in the STANDARD run is determined by BRAGFLO.

Results from each of these process steps are shown in this section. Comparisons are made between the CRA-2014 PA results at different brine volumes and the CRA-2009 PABC results. PANEL CONCENTRATION calculations run 3 replicates, but this analysis only reflects replicate 1 results. Consequently, Figures shown in Sections 5.1 and 5.3 are prepared for replicate 1 results. Section 5.1 presents "source term" results for Am and Pu. These results show how much Am or how much Pu could be mobilized in a liter of brine (either Salado or Castile brine) if there is adequate inventory present. PANEL calculates these values for the isotopes not shown in bold in Table 11. However, only Am and Pu are shown here. Am was chosen for discussion because it has a single oxidation state (+III), and it is important in WIPP PA results. Pu was chosen for discussion because it has two oxidation states (+III and +IV) and it is important in WIPP PA results.

Section 5.2 shows changes in the radionuclide inventory over time due to radioactive decay and production for isotopes of Am, Pu, U, Sr, Cs and other minor isotopes. PANEL calculates decayed activities for all of the isotopes in Table 11. However, these isotopes were chosen for discussion because they are important in WIPP PA, and they demonstrate most of the decay/production trends that one sees in the WIPP PA decay chains.

Section 5.3 presents calculated concentrations for the "lumped" isotopes (needed by CCDFGF for Culebra releases in S1-S5) and for the total EPA units (needed for CCDFGF DBR calculations).

Section 5.4 presents results for quantities of radionuclides up the borehole to the Culebra in the S6 scenario.

5.1 PANEL SOURCE TERM

PANEL calculated the source term for all runs. The runs used are from concentration type runs. PANEL source term results for Am and Pu are presented in Figures 2 through 23. Figures 2 through 23 are scatter plots with both the CRA-2009 PABC results (Part b in each figure) and the CRA-2014 PA results (Part a in each figure) presented. Each scatter plot shows the mobilization potential (either dissolved, humic colloid, microbial colloid, mineral fragment, intrinsic colloid or total) as the dependent variable (ordinate) in moles/liter and the sampled solubility value as the independent variable (abscissa). Table 13 provides definitions for the variables plotted in Figures 2 through 23.

Table 13. Definitions of Variables Plotted in Figures 2 through 23

Name	Type/Units	Description
AM_DIS	Moles/liter	The dissolution potential for Am
AM_HUM	Moles/liter	The mobilization potential for Am in humic colloids
AM_MIC	Moles/liter	The mobilization potential for Am in microbial colloids
AM_INT	Moles/liter	The mobilization potential for Am in intrinsic colloids
AM_MIN	Moles/liter	The mobilization potential for Am in mineral fragment colloids
AM_TMOB	Moles/liter	The total mobilization potential for Am
PU_DIS	Moles/liter	The dissolution potential for Pu
PU_HUM	Moles/liter	The mobilization potential for Pu in humic colloids
PU_MIC	Moles/liter	The mobilization potential for Pu in microbial colloids
PU_INT	Moles/liter	The mobilization potential for Pu in intrinsic colloids
PU_MIN	Moles/liter	The mobilization potential for Pu in mineral fragment colloids
PU_TMOB	dimensionless	The total mobilization potential for Pu
WSOLVAR3	dimensionless	This variable is the sampled value of the solubility variability for oxidation state III
WSOLPU	dimensionless	This variable is the sampled value of the solubility variability for Pu depending on the oxidation state of Pu

Scatter plots illustrate the range of uncertainty in each radionuclide's potential mobilized concentration. For Am, which has only one oxidation state (+III), the independent variable (the sampled value of the solubility variability for oxidation state +III) varies as the range of the uncertainty variable SOLMOD3:SOLVAR.

Figures 2 to 7 are for Am in Salado brine. Figure 2 indicates that the potential dissolved components for Am in Salado for the CRA-2014 PA decreases as the brine volume increases. The potential dissolved components for Am in Salado are similar for both the CRA-2014 PA and the CRA-2009 PABC. The gradient of the potential dissolved components for Am in Salado for the CRA-2014 PA is slightly steeper than the CRA-2009 PABC, because of the slightly increased solubility (Table 1) and a smaller uncertainty range (Table 2).

Figure 3 indicates that the range of values for the potential humic component of mobilized Am in Salado brine for the CRA-2014 PA is similar to the CRA-2009 PABC. This is to be expected since the multiplier $\left(h_{brine}^{red/ox}\right)$ in Equation 3 was not updated for the CRA-2014 PA, and the potential dissolved component (which is part of Equation 3) did change slightly (see Figure 2). It is also interesting to note in Figure 3 that the humic colloid component did reach the maximum value [$\left(H_{elem}^{\max}\right)$ in Equation 3] in both the CRA-2014 PA and the CRA-2009 PABC. This is apparent on the far right-hand-side of Figure 3 where the vectors have values equivalent to the maximum, 1.10E-05 moles/liter.

Figure 4 indicates the mobilization potential of microbial colloids. It reveals that few potential of microbial colloids for Am nonzero data points for the CRA-2014 PA exist, compared to the CRA-2009 PABC. The main reason is that the maximum concentration value for microbial colloids for Am has been significantly changed from 1.0 to 3.1E-08. This explains the largely reduced potential presence of microbial colloids compared to the CRA-2009 PABC.

Figure 5 indicates the mobilization potential of intrinsic colloids. For the CRA-2009 PABC, there were no intrinsic colloids in Salado brine since no actinide concentration of mobile actinide

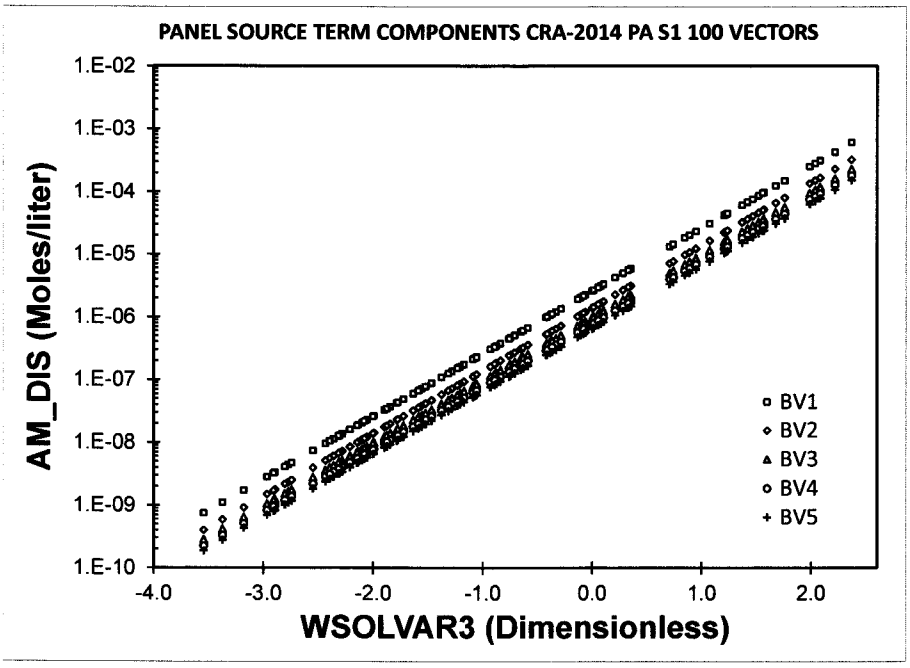
intrinsic colloids was specified in the CCA. However, the CRA-2014 PA reveals that there exists potential of intrinsic colloids for Am at 4.0E-09 moles/liter, independent upon size of brine volume (Roselle, 2013).

Figure 6 indicates that the mobilization potential for mineral fragments for Am did not change from the CRA-2009 PABC to the CRA-2014 PA. It has a constant value of 2.60E-08 moles/liter.

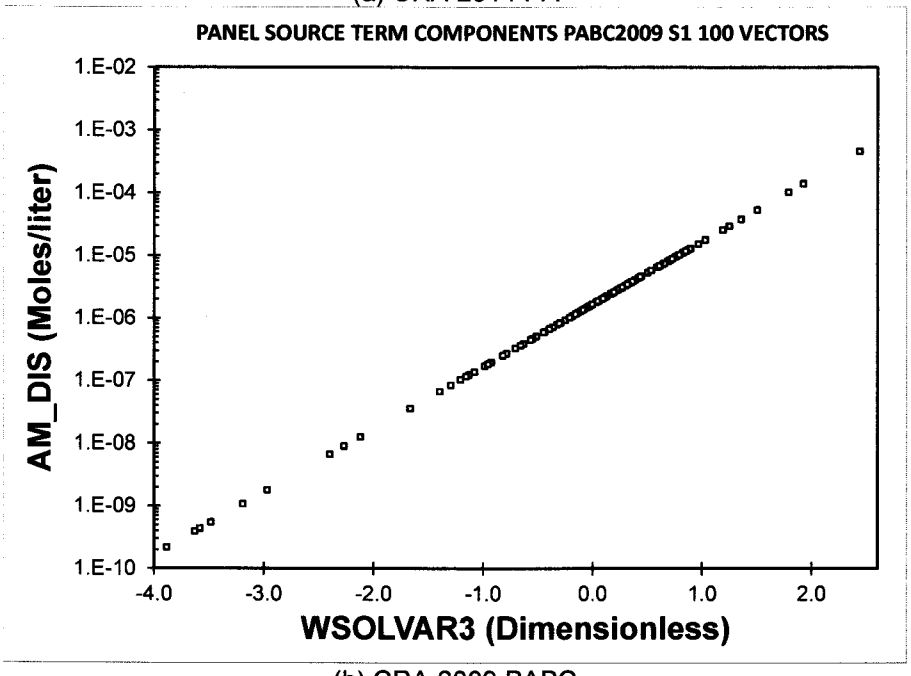
Figure 7 shows the total mobilization potential for Am in Salado brine. Value changes in mobilization potentials (dissolved, humic colloids, microbial colloids, mineral fragment colloid, and intrinsic colloids) for Am in Salado brine between the CRA-2014 PA and CRA-2009 PABC are not noticeable, and so total mobilization potentials for Am in Salado brine for the CRA-2014 PA are comparable to those for the CRA-2009 PABC.

Figures 8 to 13 are for Am in Castile brine. Most of the same conclusions that were drawn above for Am in Salado brine can be drawn as well for Am in Castile brine. The same trends are apparent. The most notable exception is shown in Figures 9 and 13. Figure 9 shows the mobilization potential for humic colloids for Am in Castile brine. In this particular case, the value of $\left(h_{brine}^{red/ox}\right)$ in Equation 3 is not a constant but is instead a sampled variable (see Table 6). The result is more "scatter" in the figure. Figure 9 also shows that humic colloids can reach the maximum value of 1.1E-05 moles/liter in both the CRA-2014 PA and the CRA-2009 PABC. In Figure 13, both Part (a) and Part (b) shows a fairly continuous curve.

The scatter seen in Figure 9 for the Am humic colloid component in Castile brine causes some scatter in Figure 13 which is the total mobilization potential for Am in Castile brine.

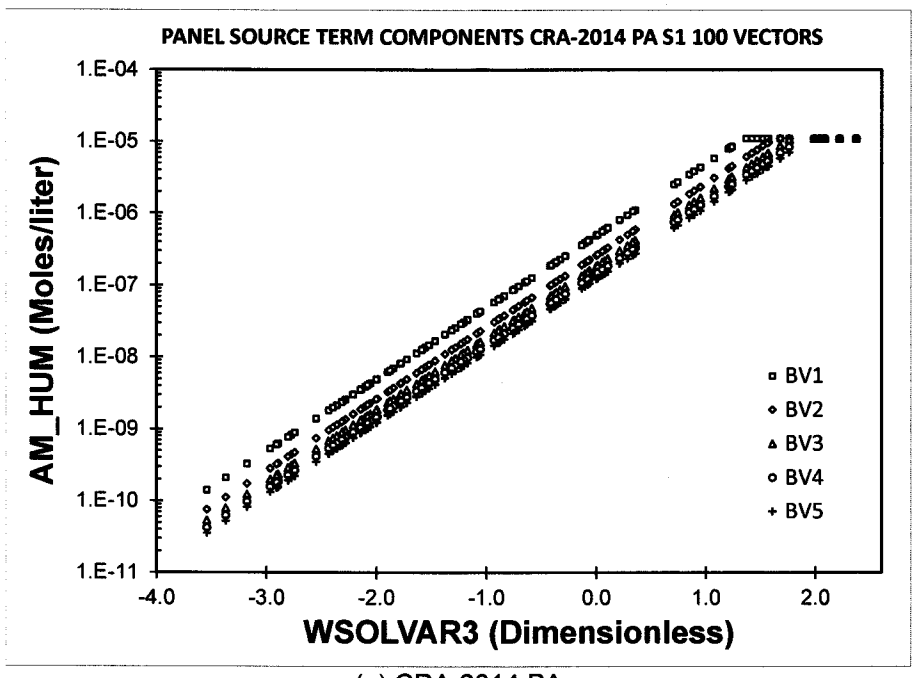


(a) CRA-2014 PA

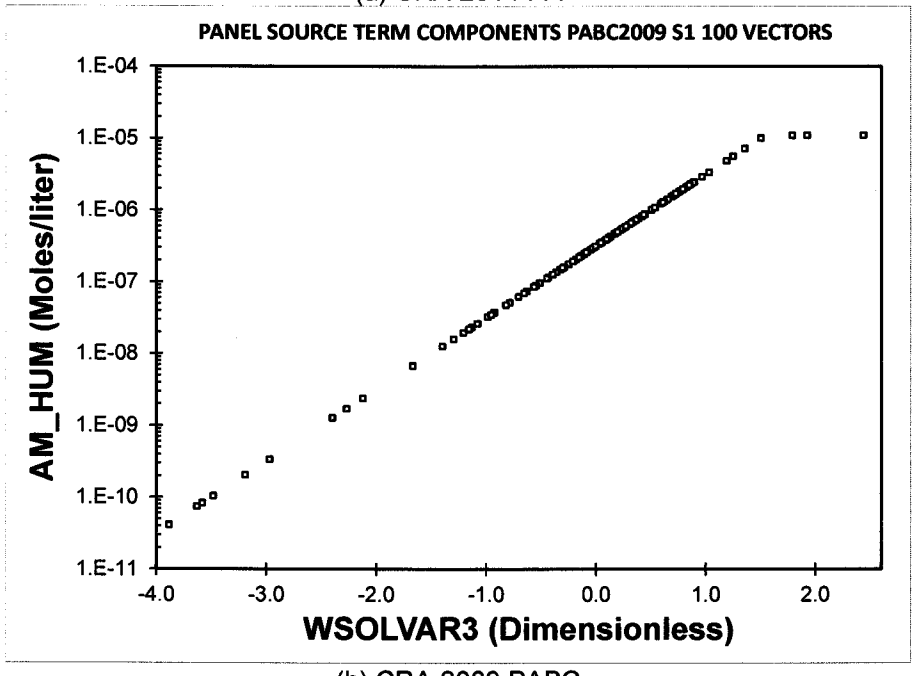


(b) CRA-2009 PABC

Figure 2. Scatter Plot of Dissolution Potential for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

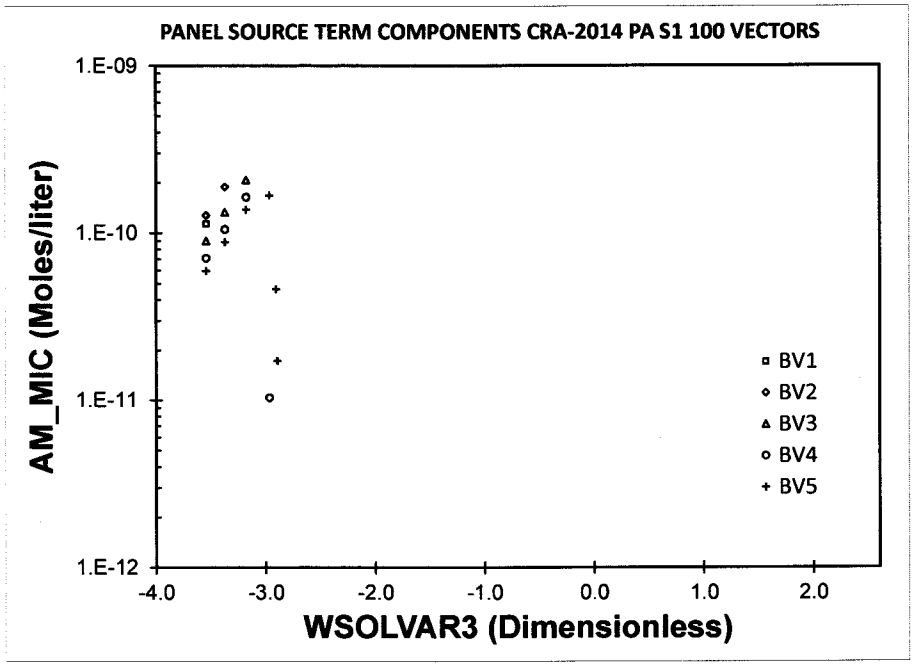


(a) CRA-2014 PA

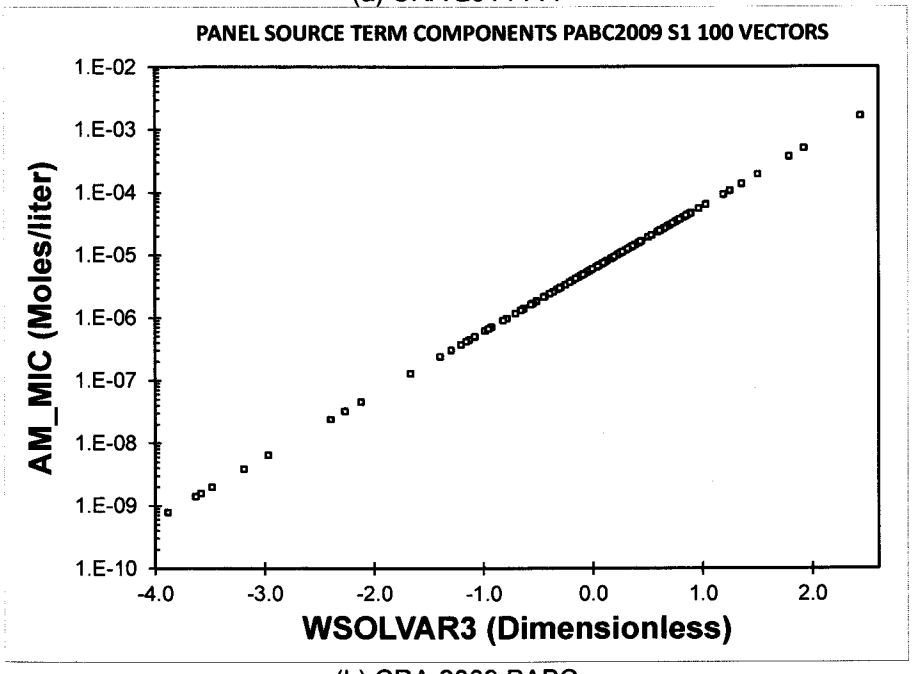


(b) CRA-2009 PABC

Figure 3. Scatter Plot of Potential Humic Colloid Component for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

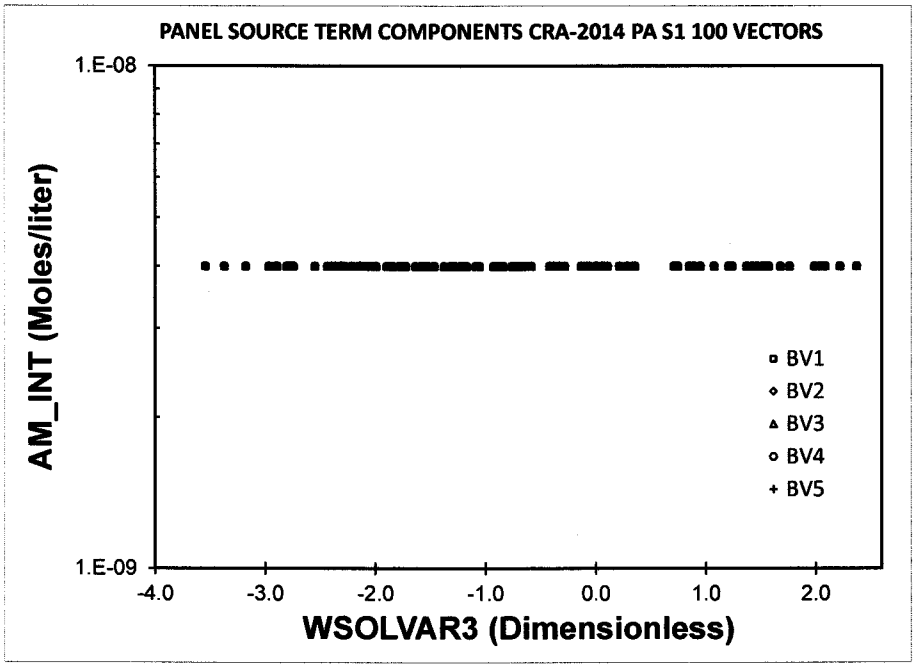


(a) CRA-2014 PA



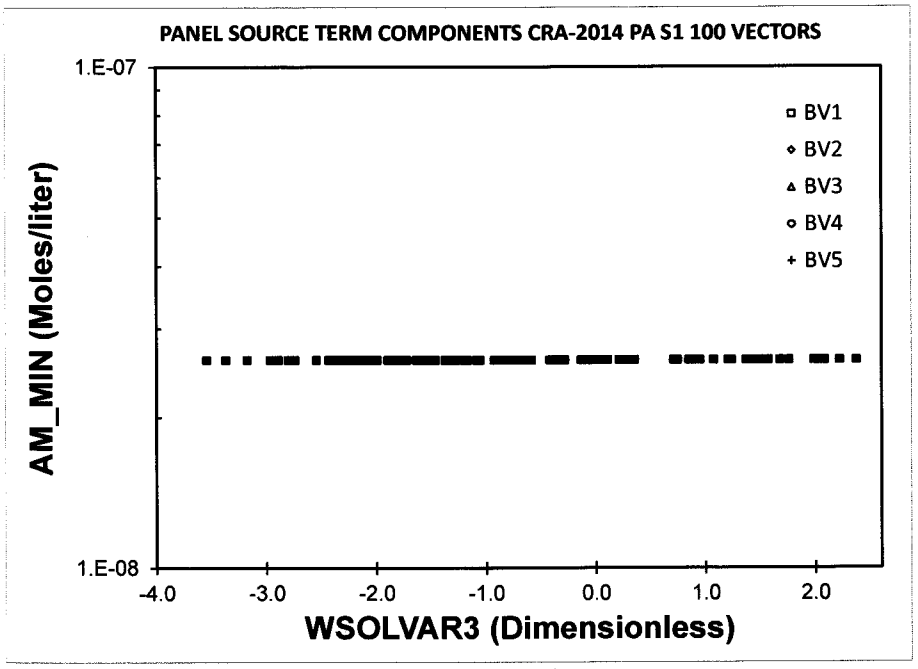
(b) CRA-2009 PABC

Figure 4. Scatter Plot of Mobilization Potential for Microbial Colloids for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

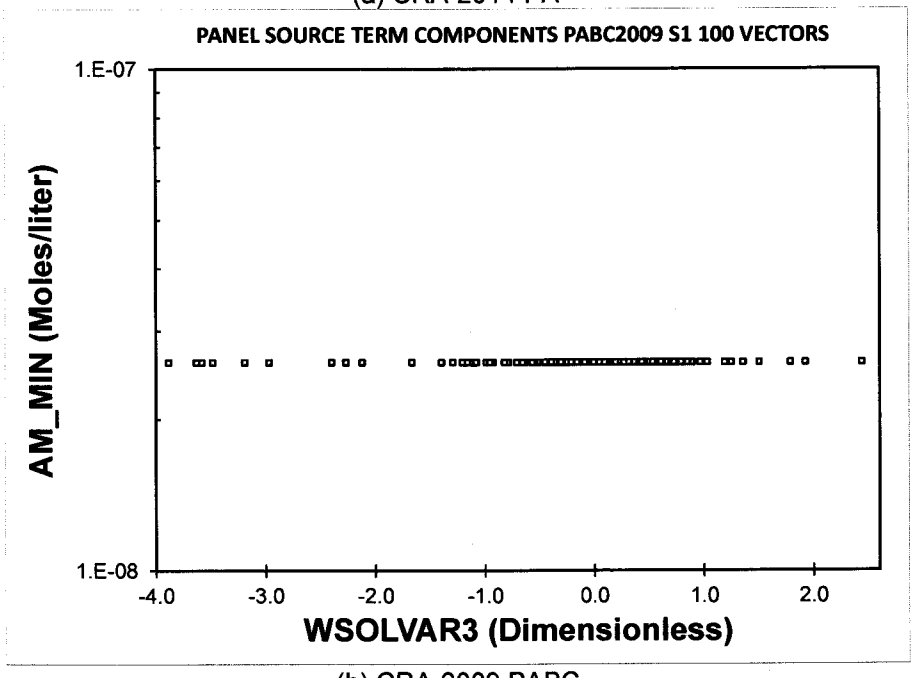


(a) CRA-2014 PA

Figure 5. Scatter Plot of Mobilization Potential for Intrinsic Colloids for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Results came from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV).

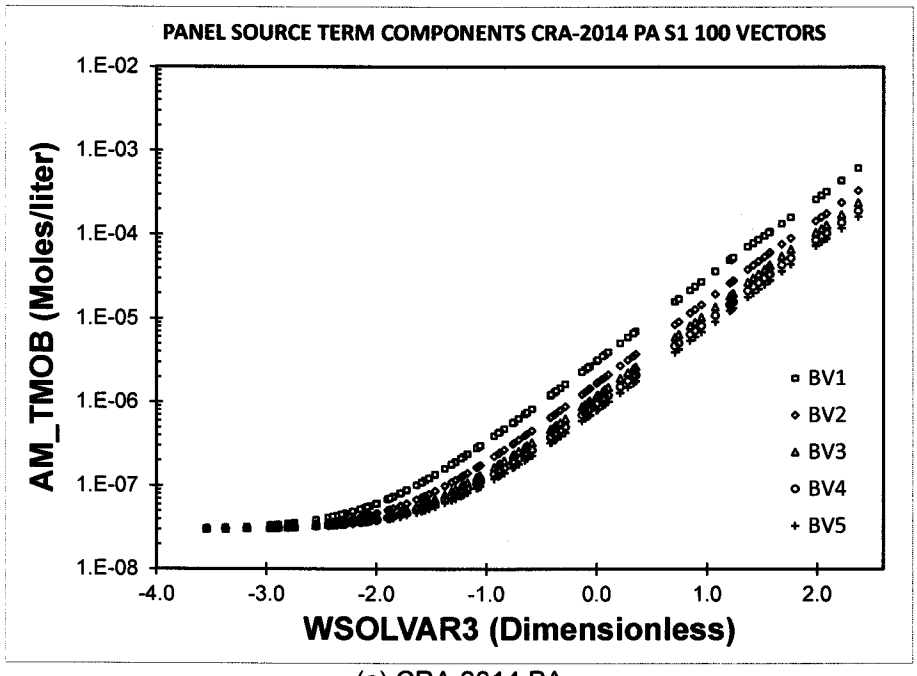


(a) CRA-2014 PA

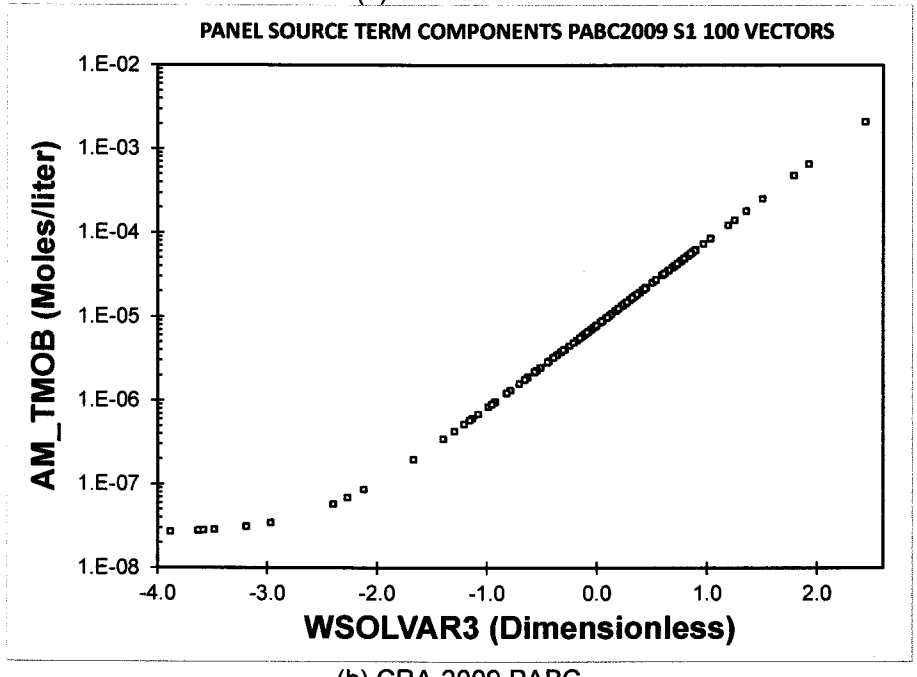


(b) CRA-2009 PABC

Figure 6. Scatter Plot of Mobilization Potential for Mineral Fragments for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

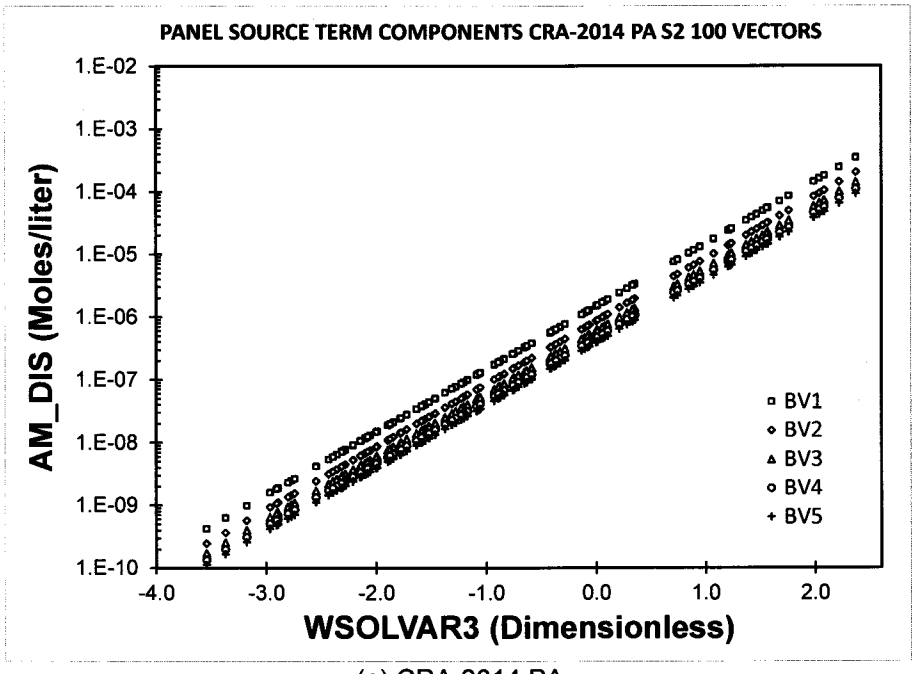


(a) CRA-2014 PA

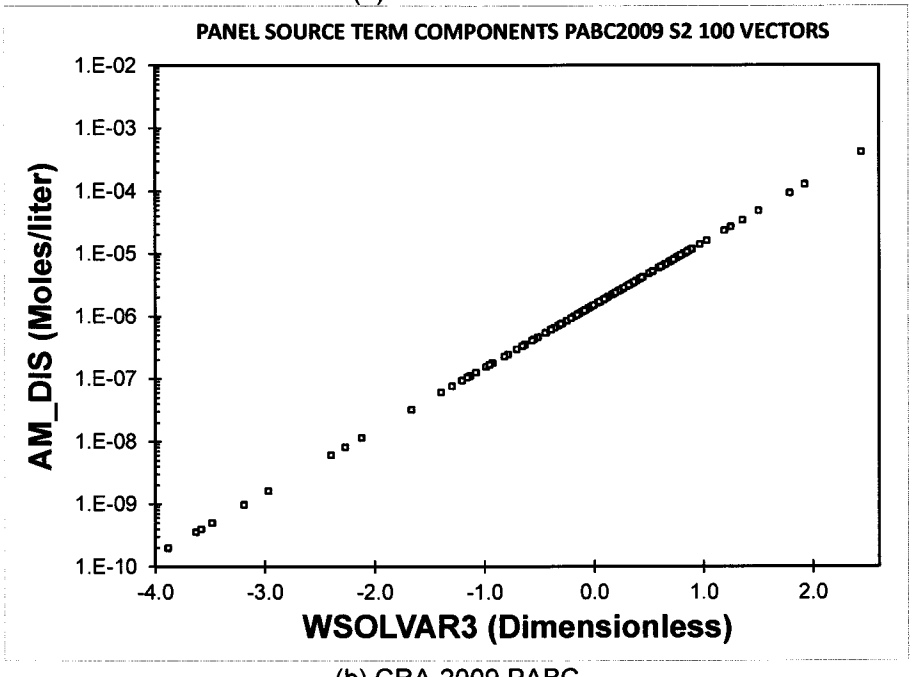


(b) CRA-2009 PABC

Figure 7. Scatter Plot of Total Mobilization Potential for Am in Salado Brine. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

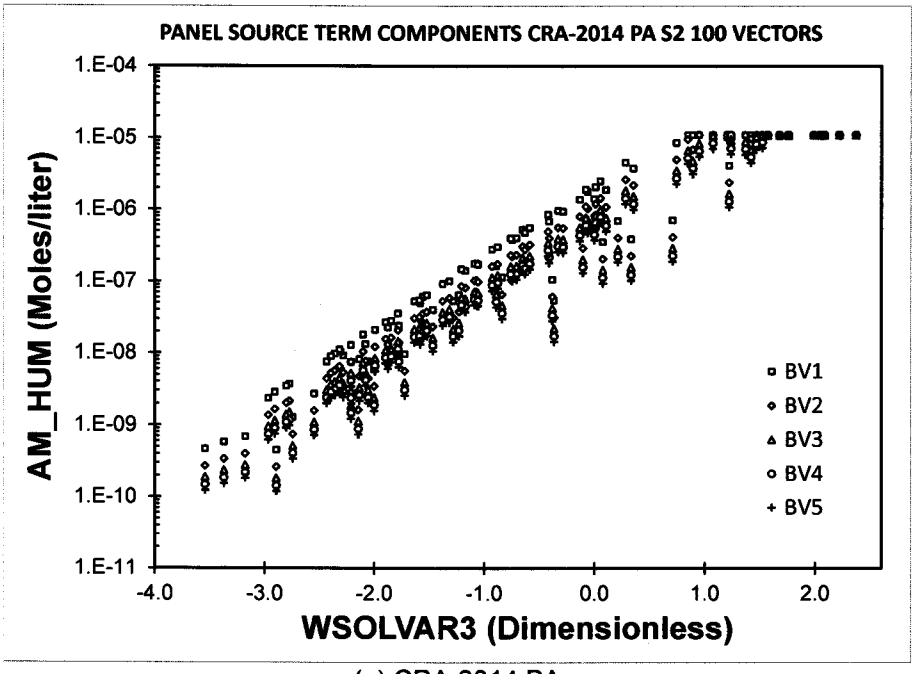


(a) CRA-2014 PA

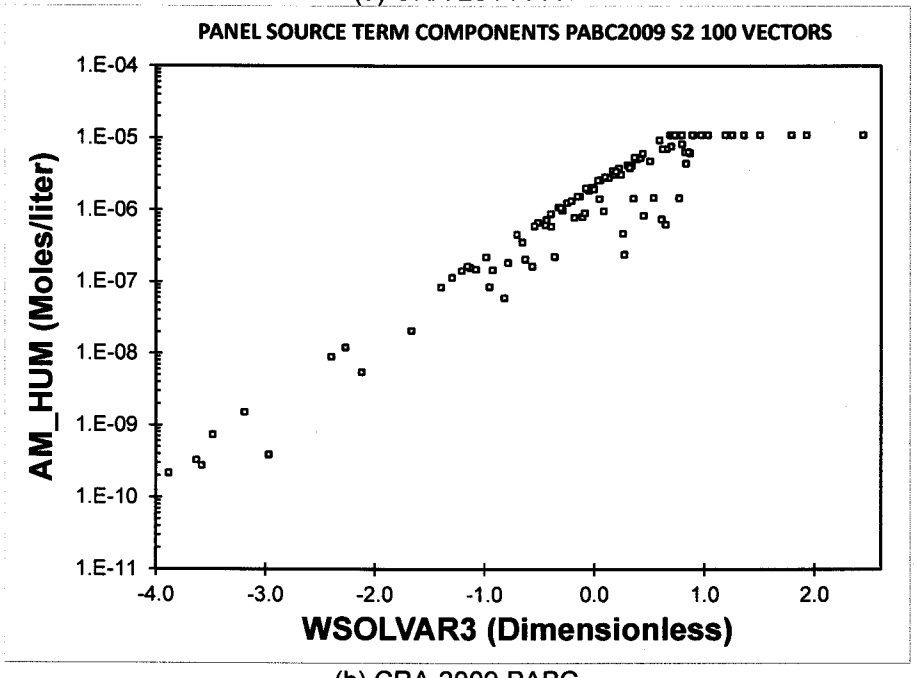


(b) CRA-2009 PABC

Figure 8. Scatter Plot of Dissolution Potential for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

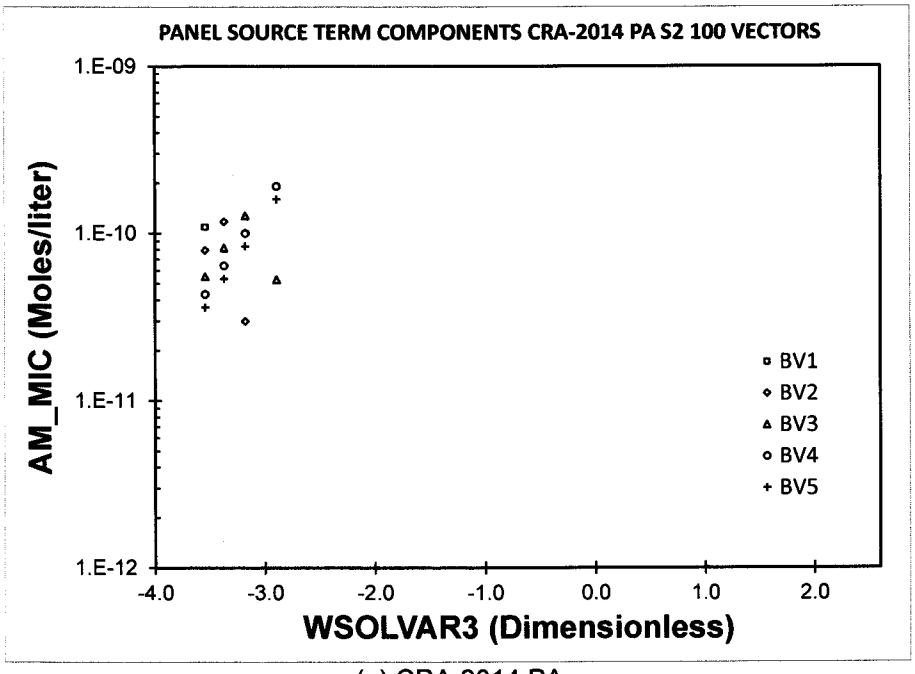


(a) CRA-2014 PA

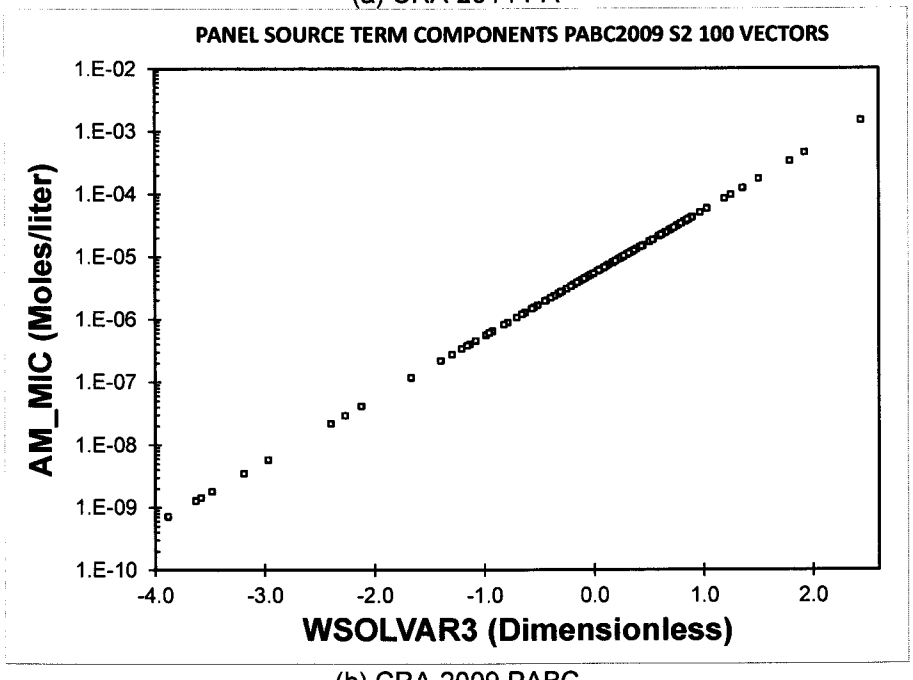


(b) CRA-2009 PABC

Figure 9. Scatter Plot of Mobilization Potential for Humic Colloids for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

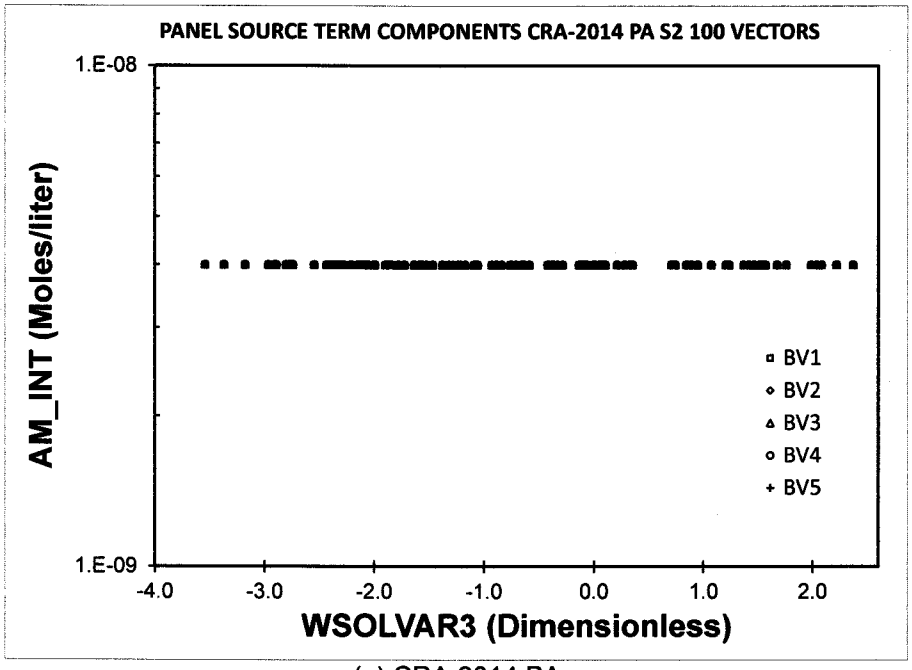


(a) CRA-2014 PA



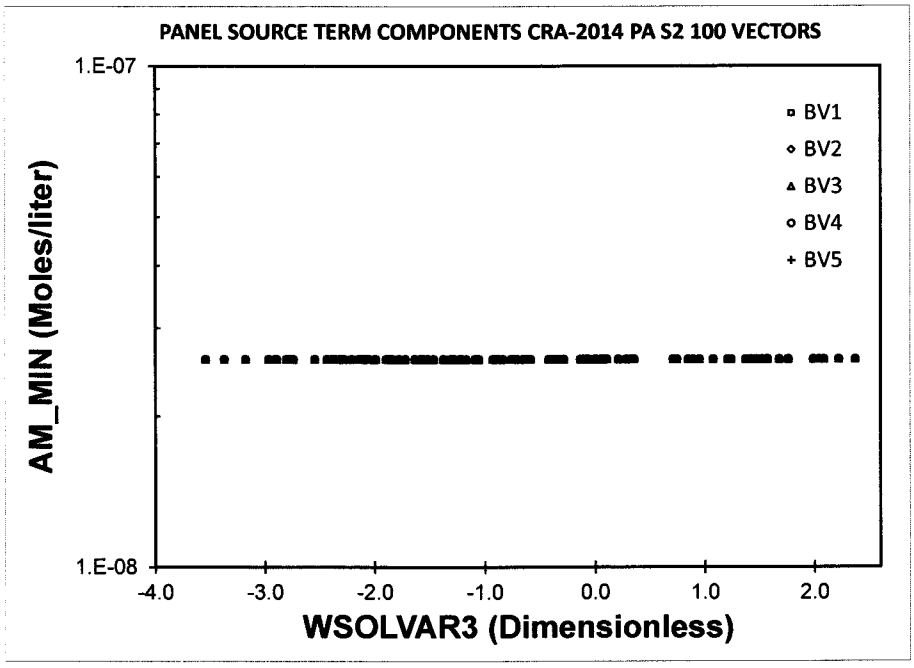
(b) CRA-2009 PABC

Figure 10. Scatter Plot of Mobilization Potential for Microbial Colloids for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

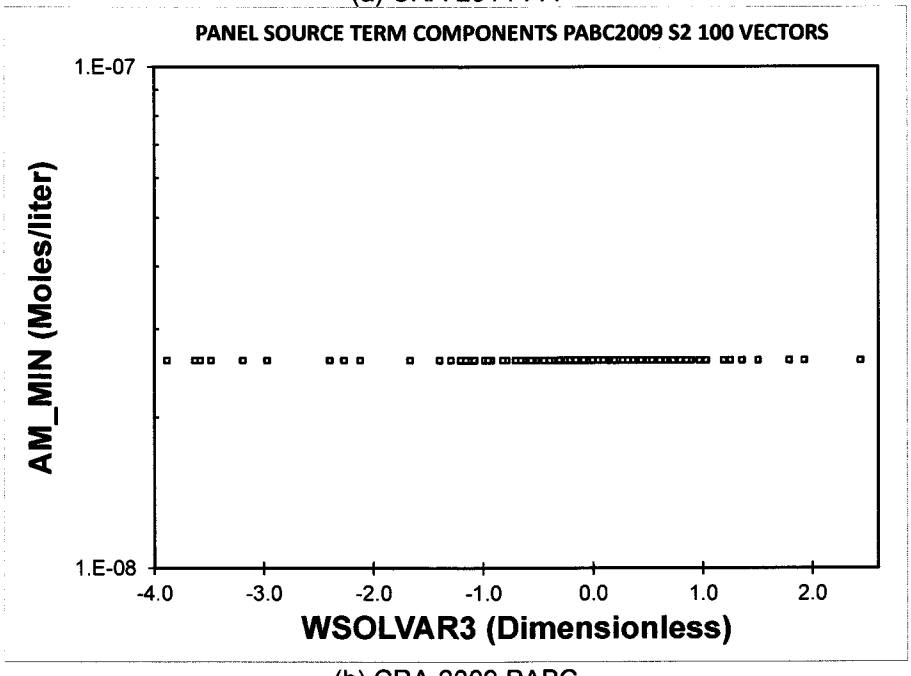


(a) CRA-2014 PA

Figure 11. Scatter Plot of Mobilization Potential for Intrinsic Colloids for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Results came from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV).

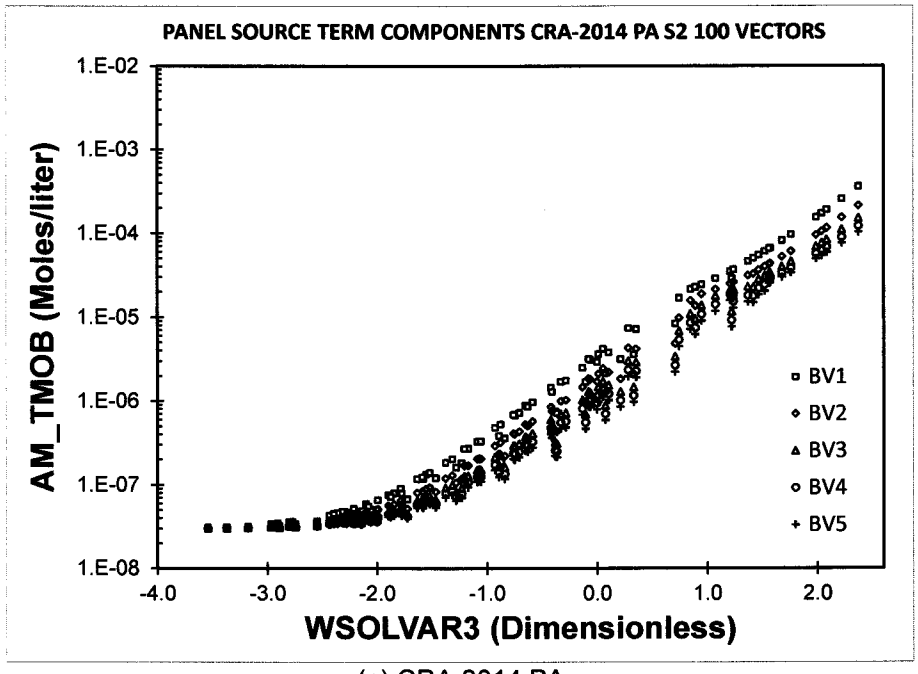


(a) CRA-2014 PA

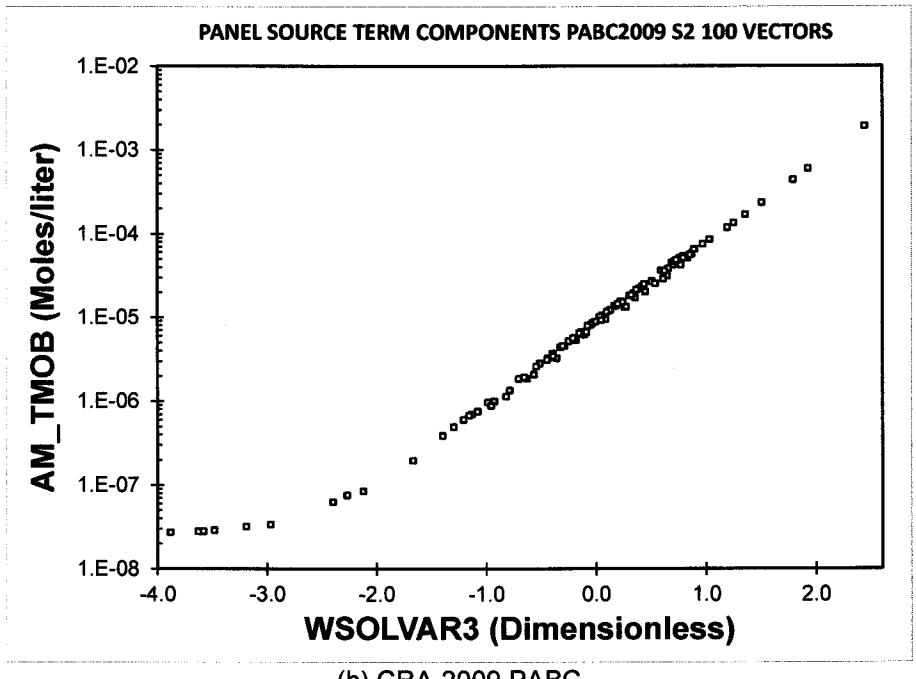


(b) CRA-2009 PABC

Figure 12. Scatter Plot of Mobilization Potential for Mineral Fragments for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.



(a) CRA-2014 PA



(b) CRA-2009 PABC

Figure 13. Scatter Plot of Total Mobilization Potential for Am in Castile Brine. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

In WIPP PA, Pu can occur in either oxidation state +III or +IV, depending on the value of GLOBAL:OXSTAT (see Table 2) which is sampled from a uniform distribution between 0 and 1. If GLOBAL:OXSTAT is less than or equal to .5, Pu will be in oxidation state +III. If it is greater than .5, the oxidation state for Pu will be +IV.

PANEL source term results for Pu are presented in Figures 14 through 25. Figures 14 to 19 are for Pu in Salado brine. Figures 20 to 25 are for Pu in Castile brine. Most of these figures show at least two distinct sets of data, one that corresponds to Pu in the +III oxidation state and one that corresponds to Pu in the +IV oxidation state. The exceptions are Figures 17, 18, 23 and 24 showing the mobilization potential for intrinsic and mineral fragments colloids which are constant values (see Equations 4 and 5) and independent of oxidation state. Another exception is Figure 15 showing the mobilization potential for humic colloids in Salado brine, though that in Castile brine depends on oxidation state. It should be noted that the mobilization potential for humic colloids in Salado brine for the CRA-2009 PABC depends on oxidation state (Garner, 2010).

In the figures where two sets of data are shown (Figures 14, 16, 19-22, 25), the upper set of data corresponds to Pu in the +III oxidation state. These results are essentially identical to those for Am in the +III oxidation state. The lower set of data corresponds to Pu in the +IV oxidation state. An(IV) solubility (SOLMOD4) for the CRA-2014 PA (Table 1) shows a consistent value independent of various brine volumes. Based on Equations (2), (3), (6), and (7), this leads the mobilization potentials for Pu(IV) show no impact from brine volume changes. To distinguish mobilization potentials for Pu(IV) from Pu(III), oxidation state of Pu(IV) is labeled on Part (a) in Figure 14 - 16, 19 - 22, and 25.

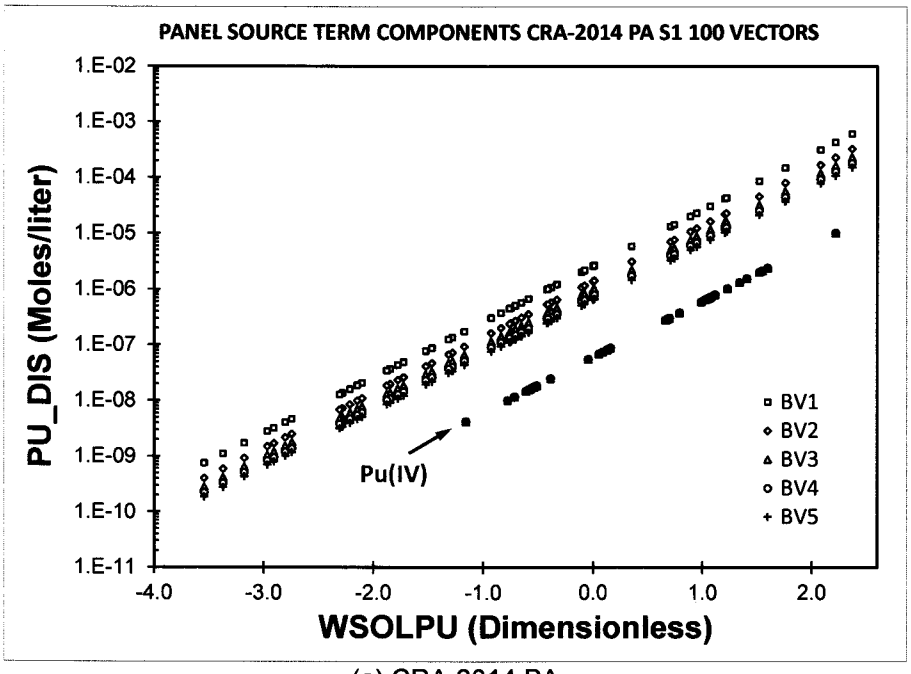
Figure 14 and Figure 20 show the dissolution potential for Pu in Salado brine and Castile brine, respectively. In Part (a) (CRA-2014 PA) the top curve (+III) has a larger range and depends on the brine volume. The bottom curve (+IV) has a smaller range than the CRA-2009 PABC, and is independent on size of the brine volume.

Figure 15 shows the range of values for the mobilization potential for humic colloids for Pu in Salado brine. Both Part (a) and Part (b) reach the maximum value. The CRA-2009 PABC appears as only one line since the +III Salado solubility (Table 1) times the +III Salado humic proportionality constant (Table 6) is approximately equal to the +IV Salado solubility (Table 1) times the +IV Salado humic proportionality constant (Table 6). However the CRA-2014 PA shows a distinction: the top curve (+III) lowers with the increasing brine volume, and a slightly lower curve (+IV) shows independence on various brine volumes.

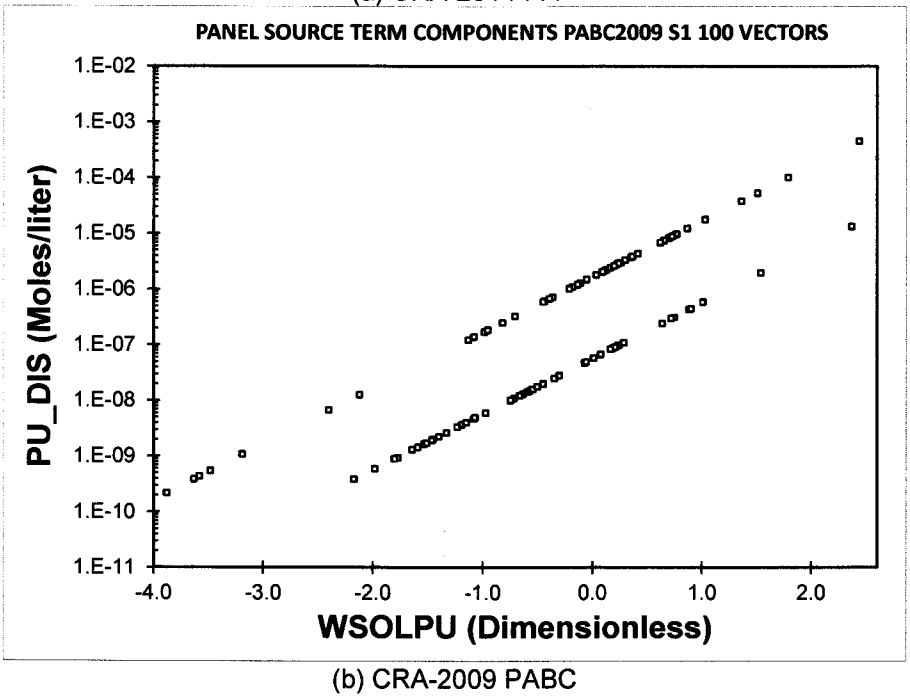
Figure 16 shows two distinct data subsets in both Part (a) (CRA-2014 PA results) and Part (b) (the CRA-2009 PABC results). The two subsets of data correspond to Pu in the two different oxidation states.

Figure 19 shows the total mobilization potential for Pu in Salado brine. Part (a) shows the CRA-2014 PA results and Part (b) shows the CRA-2009 PABC results. As addressed above, the total mobilization potential for Pu(+IV) for the CRA-2014 PA is independent on size of the brine volume. Figure 25 shows the same trend in the total mobilization potential for Pu is Castile

brine. Figure 25 is a bit nosier because of the sampled portionality factor in the +III oxidation state.

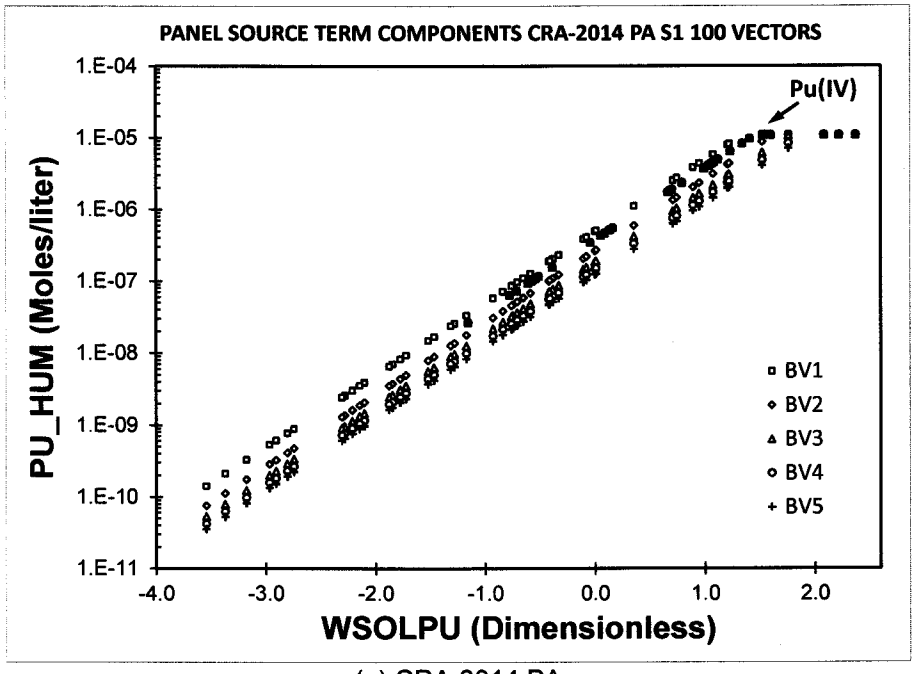


(a) CRA-2014 PA

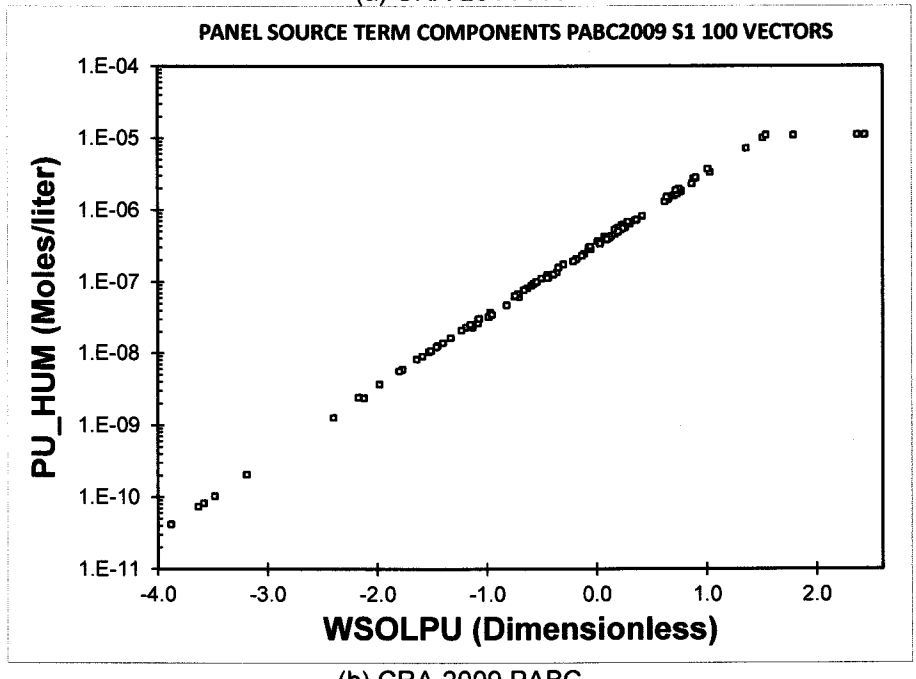


(b) CRA-2009 PABC

Figure 14. Scatter Plot of Dissolution Potential for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

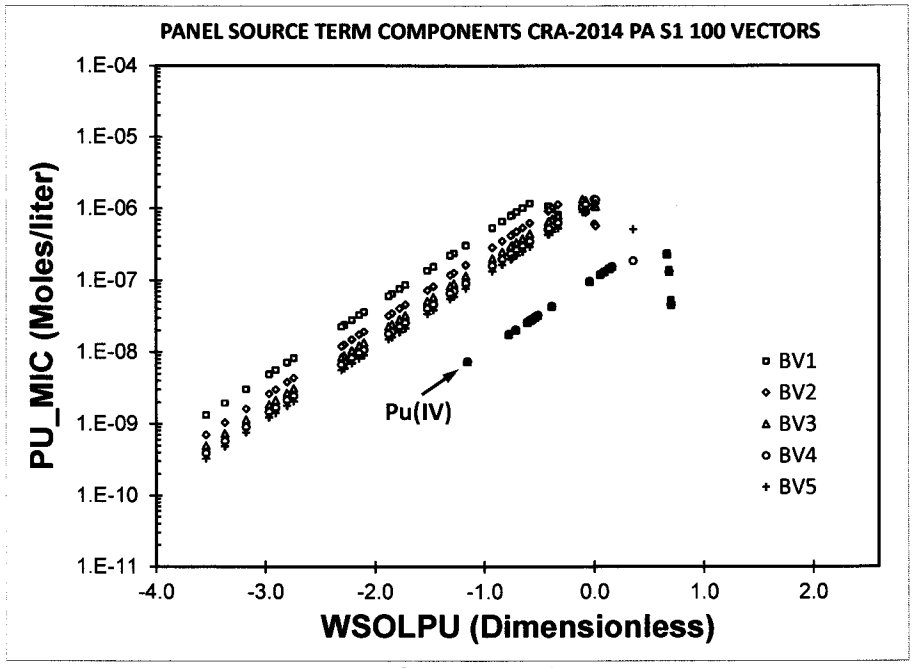


(a) CRA-2014 PA

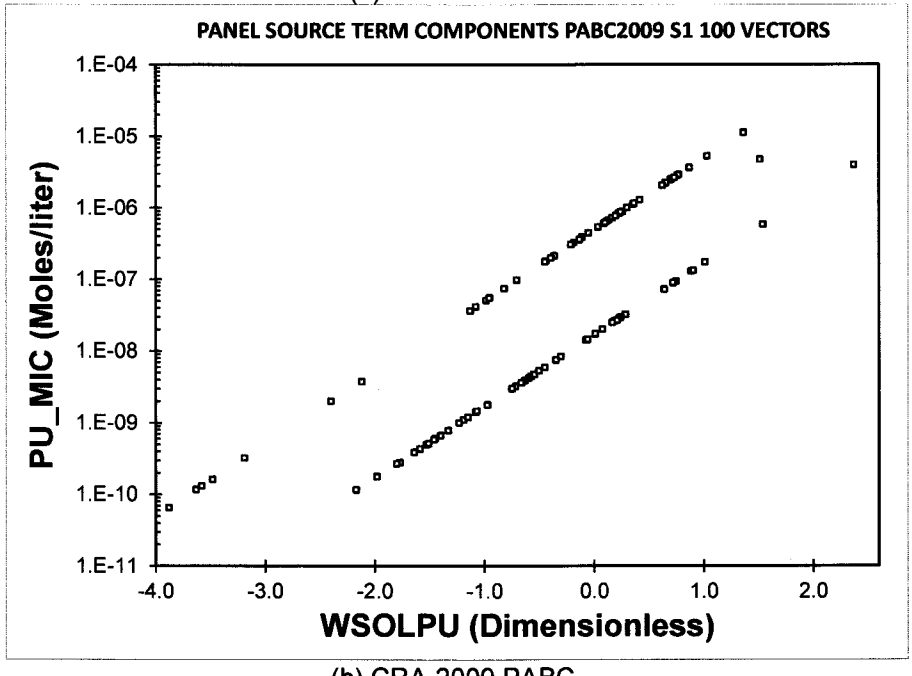


(b) CRA-2009 PABC

Figure 15. Scatter Plot of Mobilization Potential for Humic Colloids for Plutonium in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

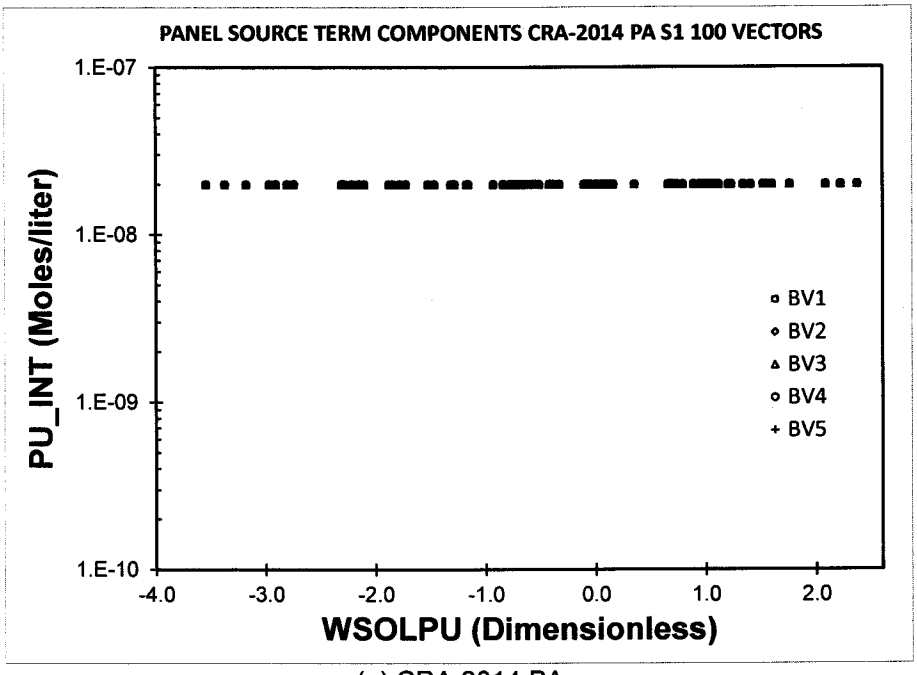


(a) CRA-2014 PA

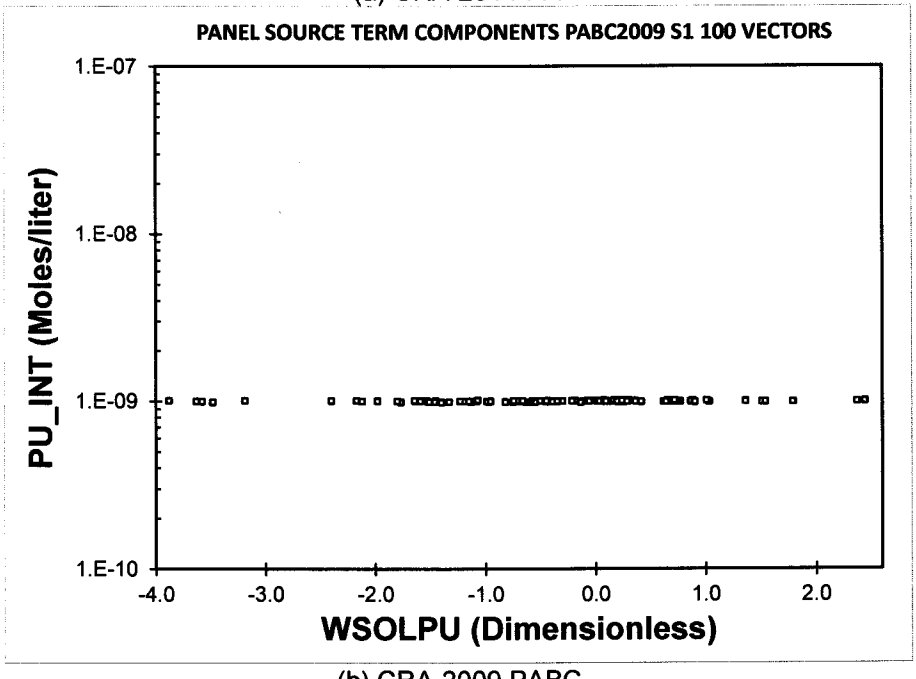


(b) CRA-2009 PABC

Figure 16. Scatter Plot of Mobilization Potential for Microbial Colloids for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

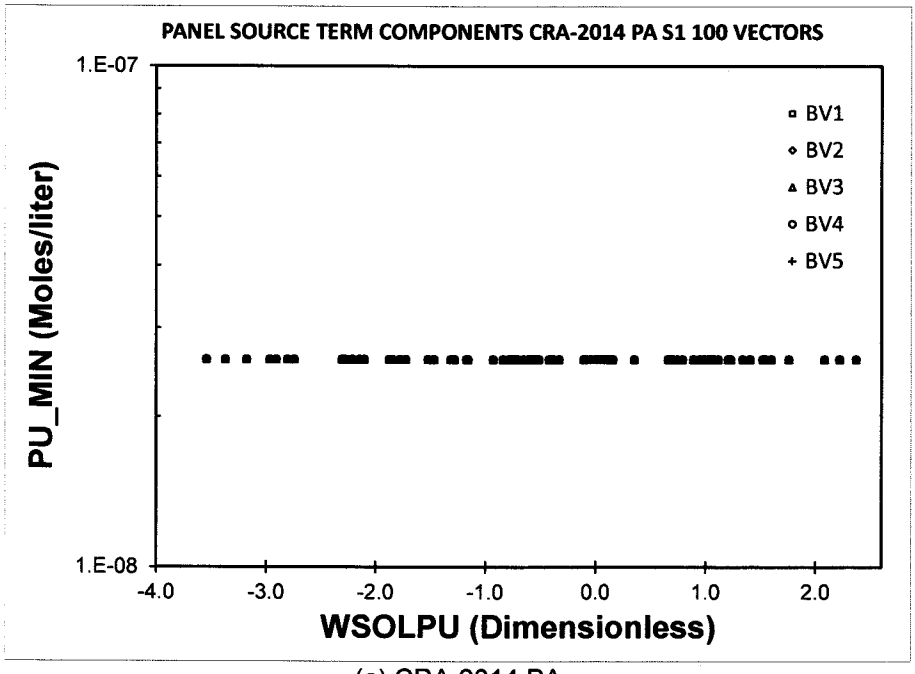


(a) CRA-2014 PA

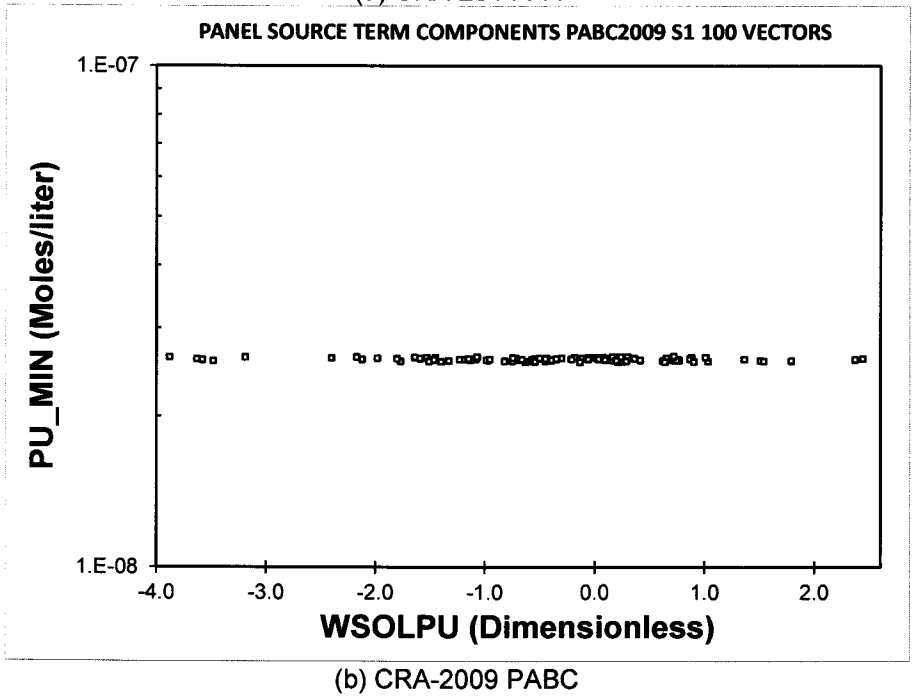


(b) CRA-2009 PABC

Figure 17. Scatter Plot of Mobilization Potential for Intrinsic Colloids for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

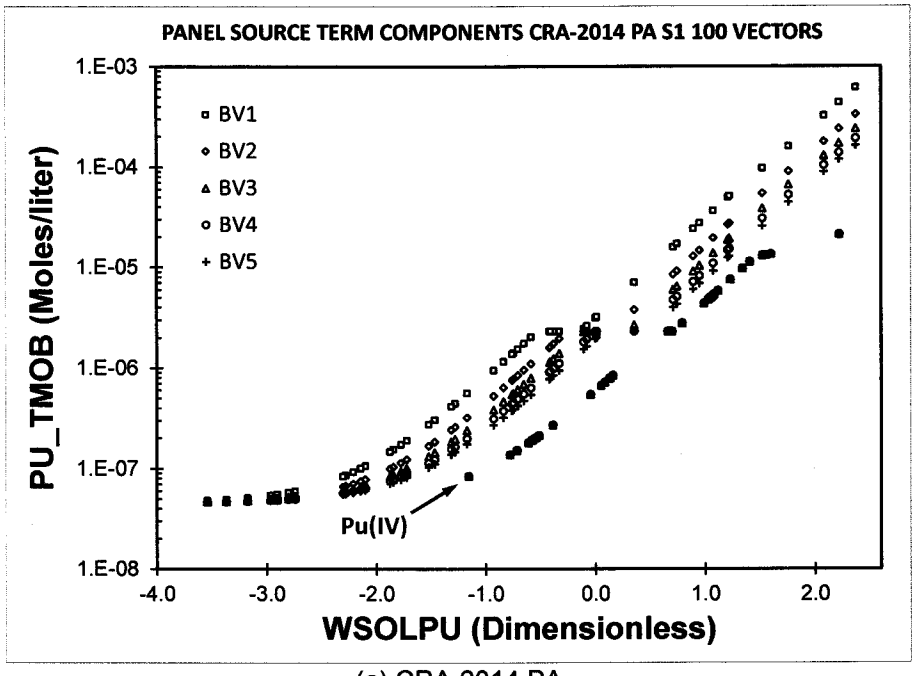


(a) CRA-2014 PA

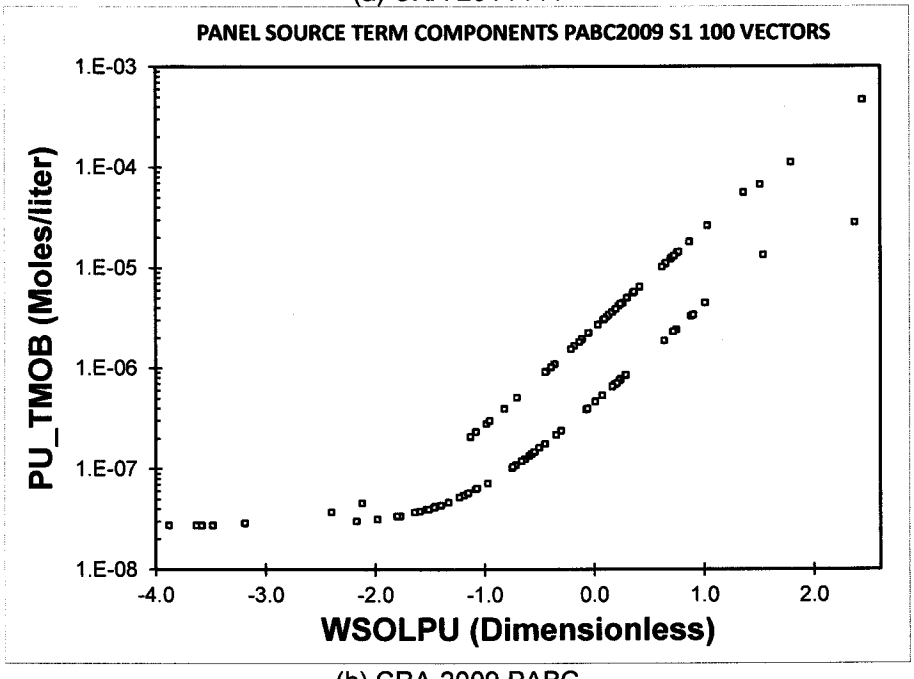


(b) CRA-2009 PABC

Figure 18. Scatter Plot of Mobilization Potential for Mineral Fragments for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

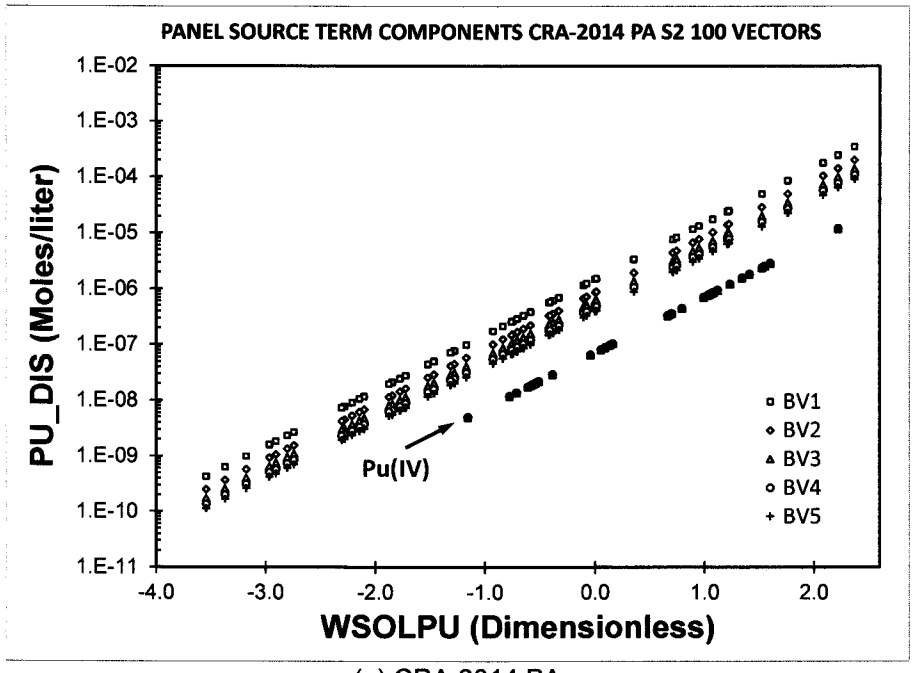


(a) CRA-2014 PA

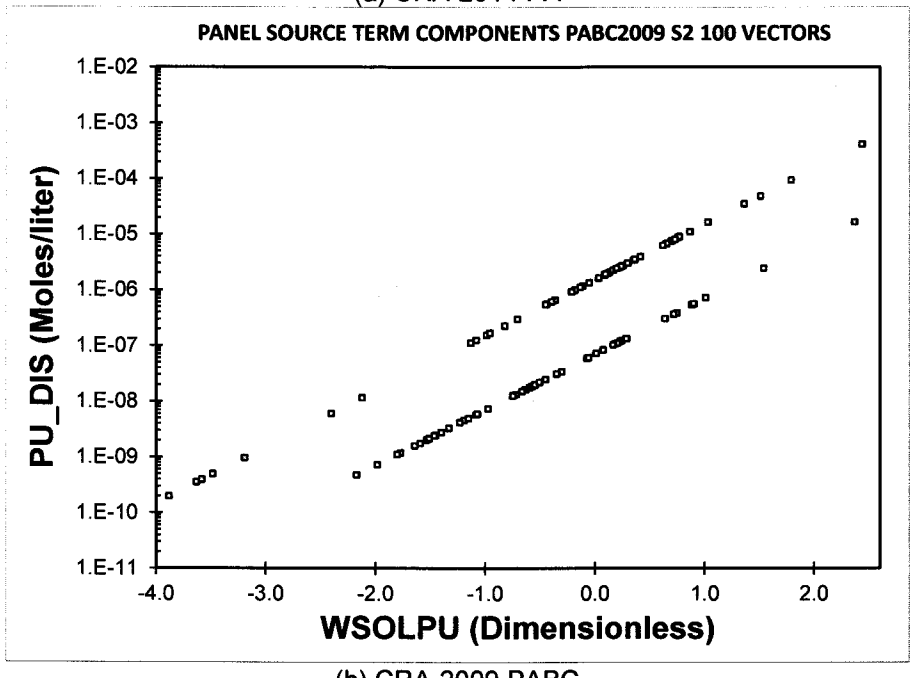


(b) CRA-2009 PABC

Figure 19. Scatter Plot of Total Mobilization Potential for Pu in Salado Brine. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

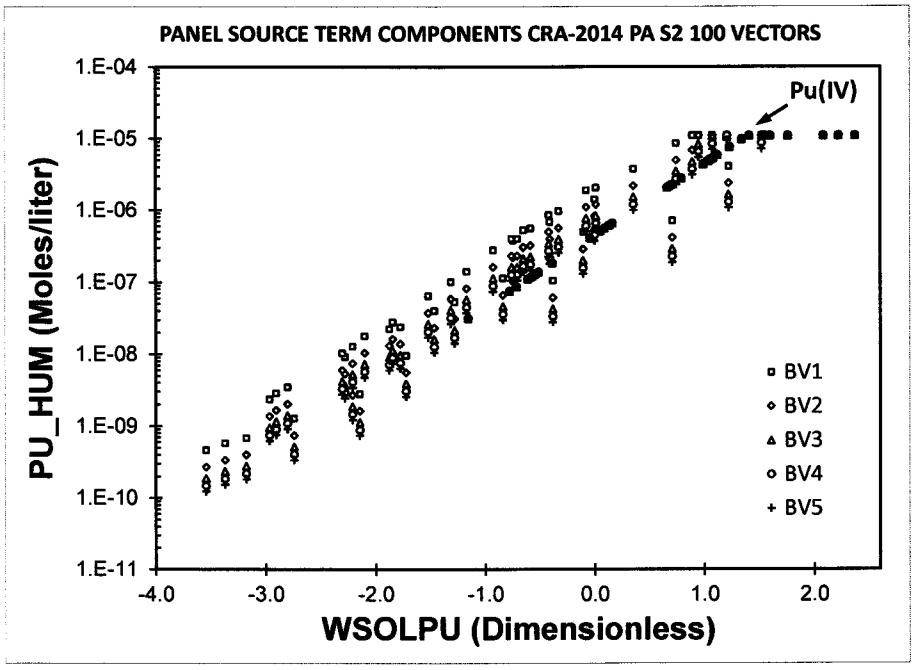


(a) CRA-2014 PA

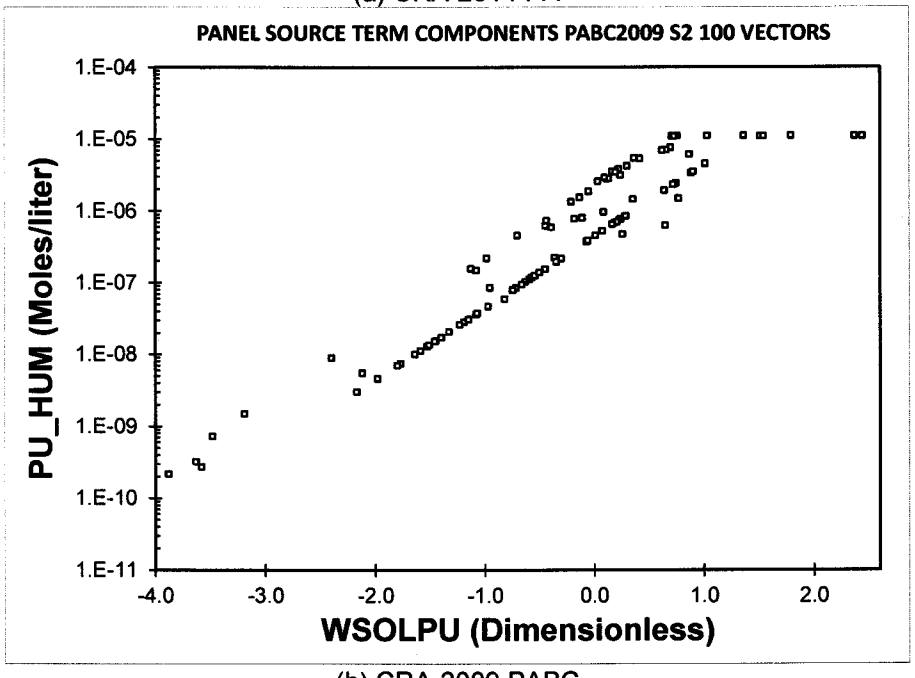


(b) CRA-2009 PABC

Figure 20. Scatter Plot of Dissolution Potential for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

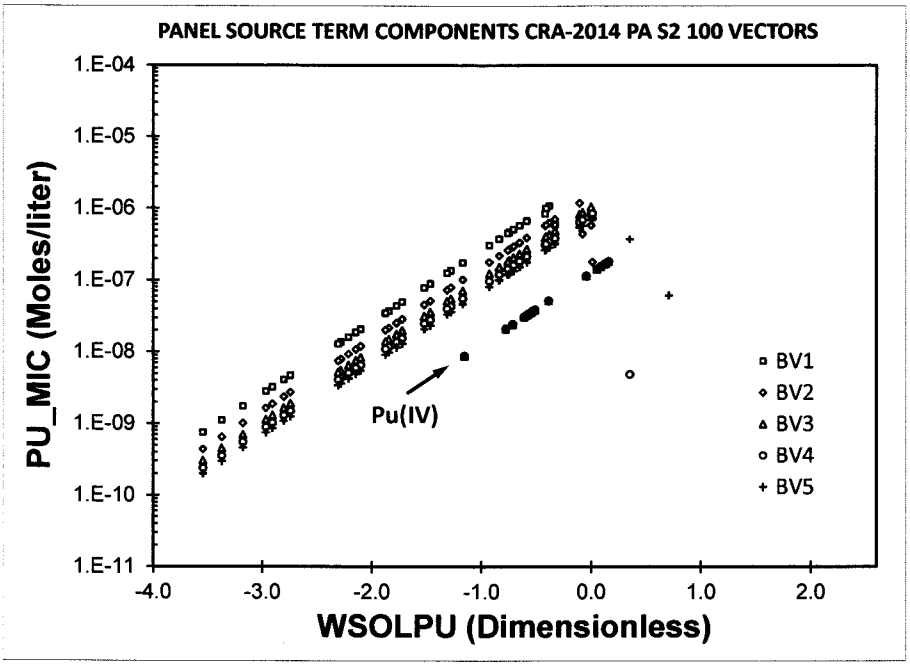


(a) CRA-2014 PA

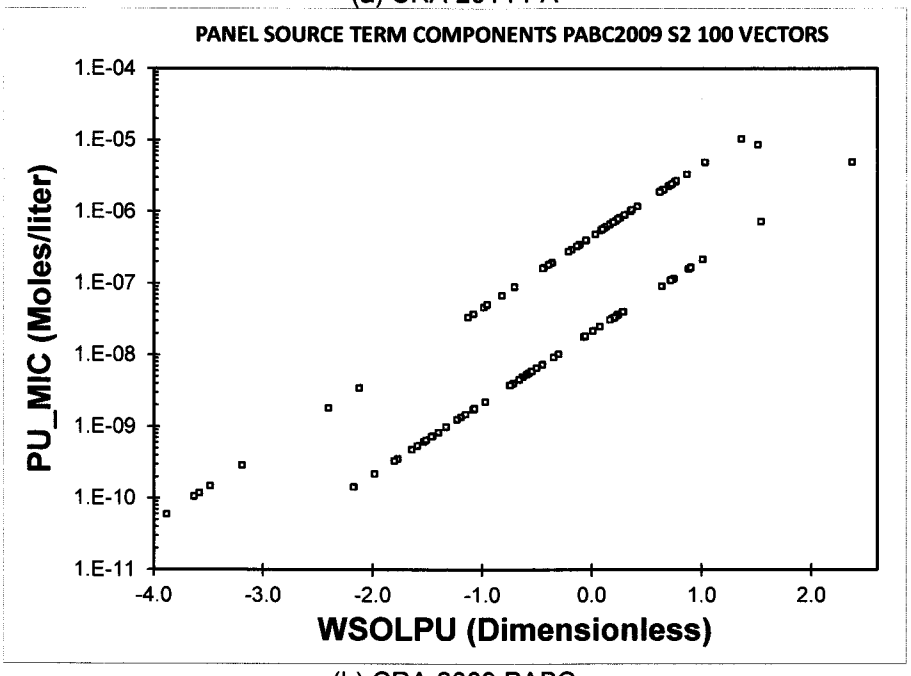


(b) CRA-2009 PABC

Figure 21. Scatter Plot of Mobilization Potential for Humic Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

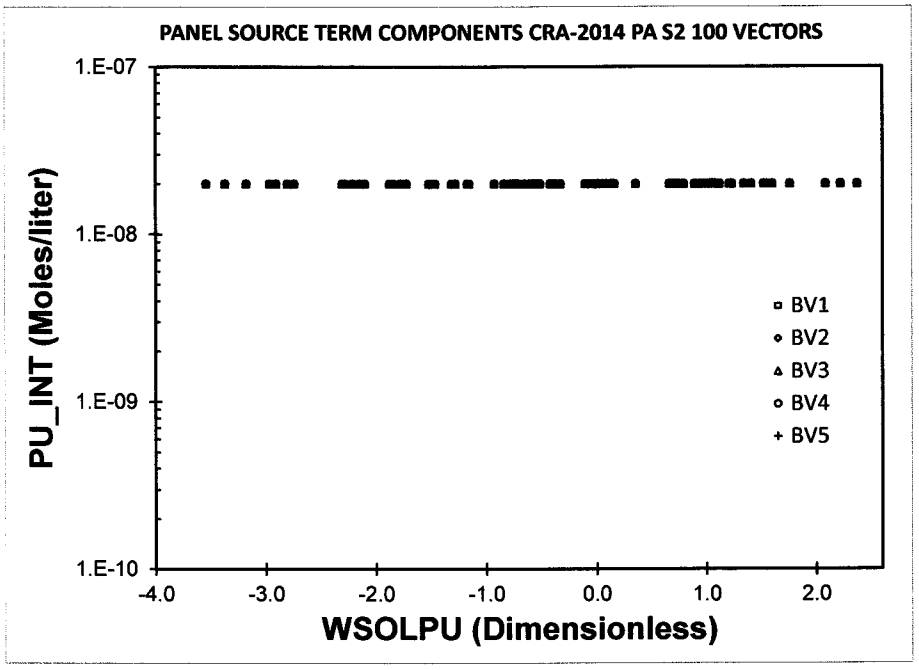


(a) CRA-2014 PA

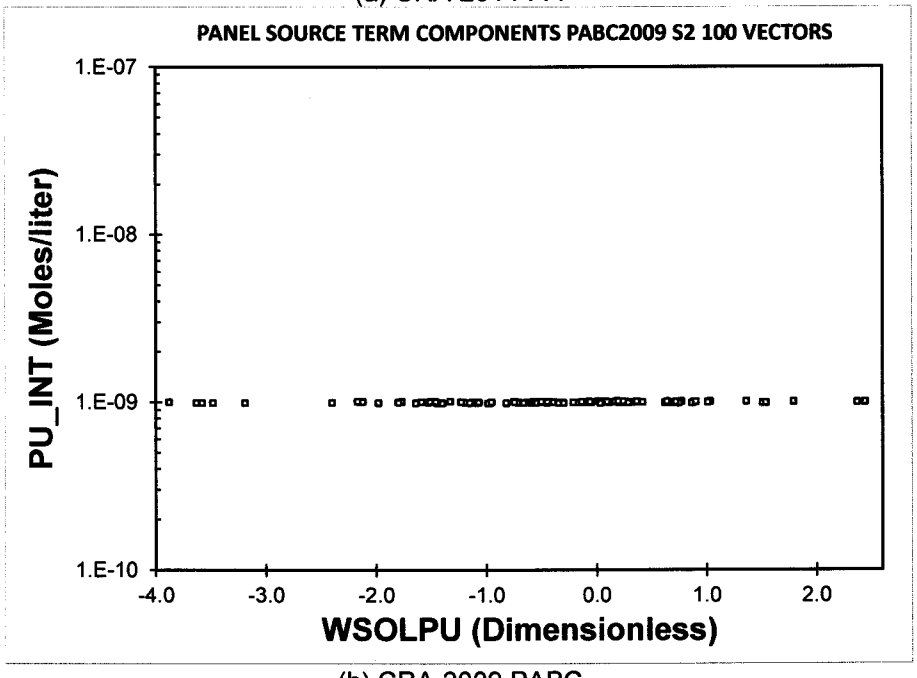


(b) CRA-2009 PABC

Figure 22. Scatter Plot of Mobilization Potential for Microbial Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

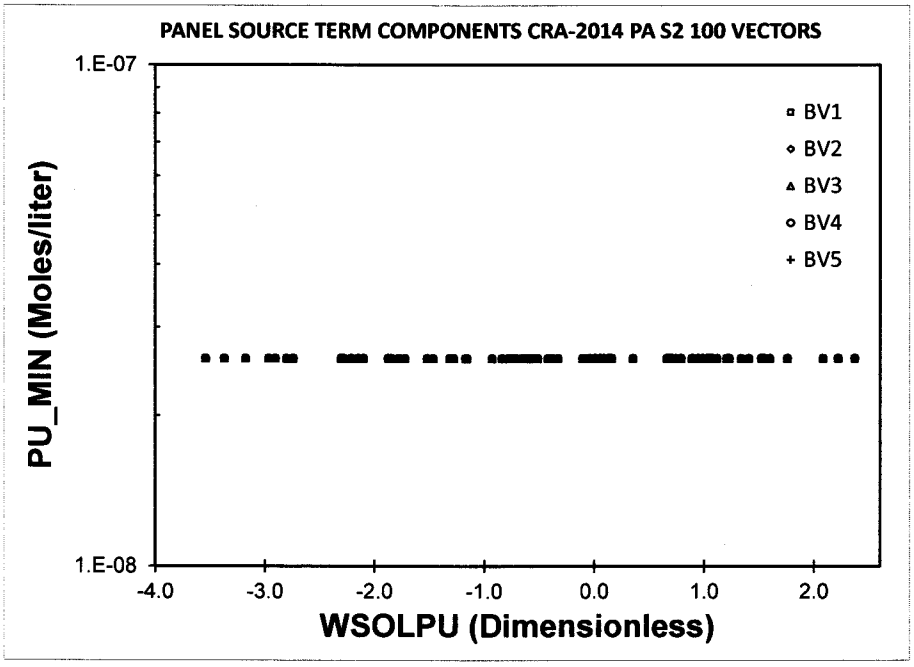


(a) CRA-2014 PA

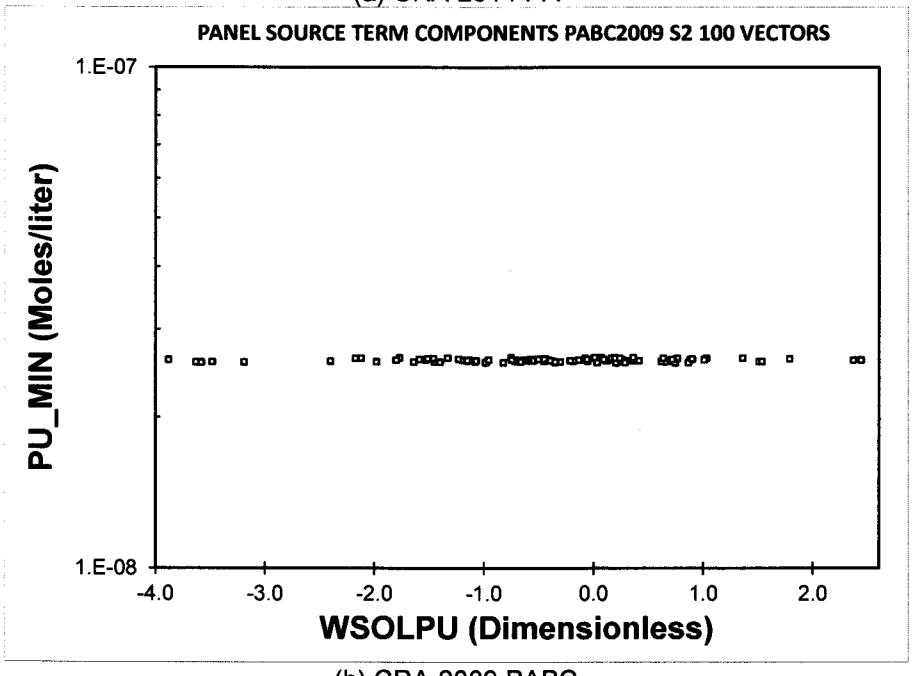


(b) CRA-2009 PABC

Figure 23. Scatter Plot of Mobilization Potential for Intrinsic Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

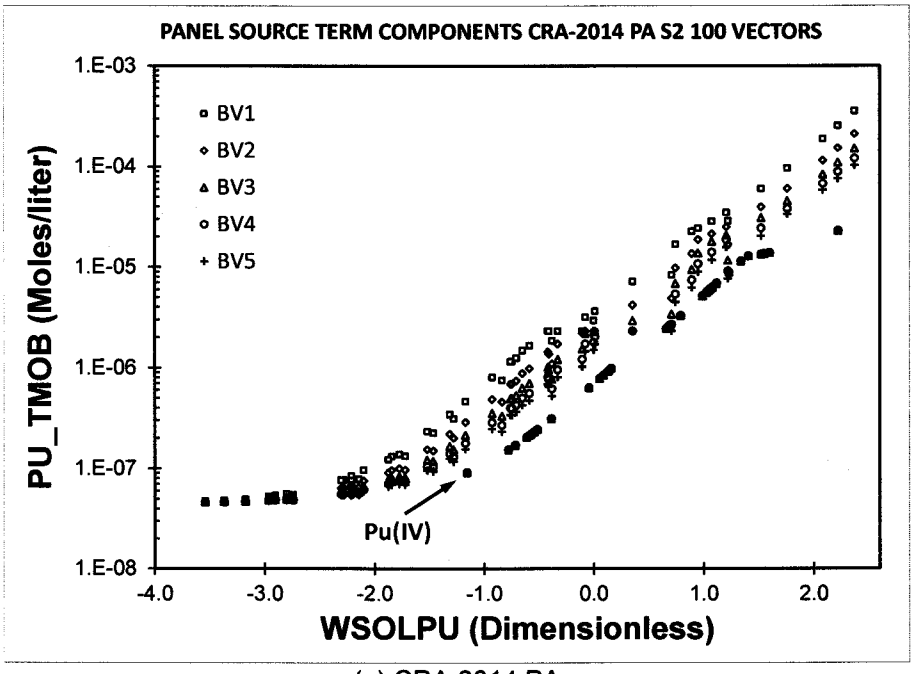


(a) CRA-2014 PA

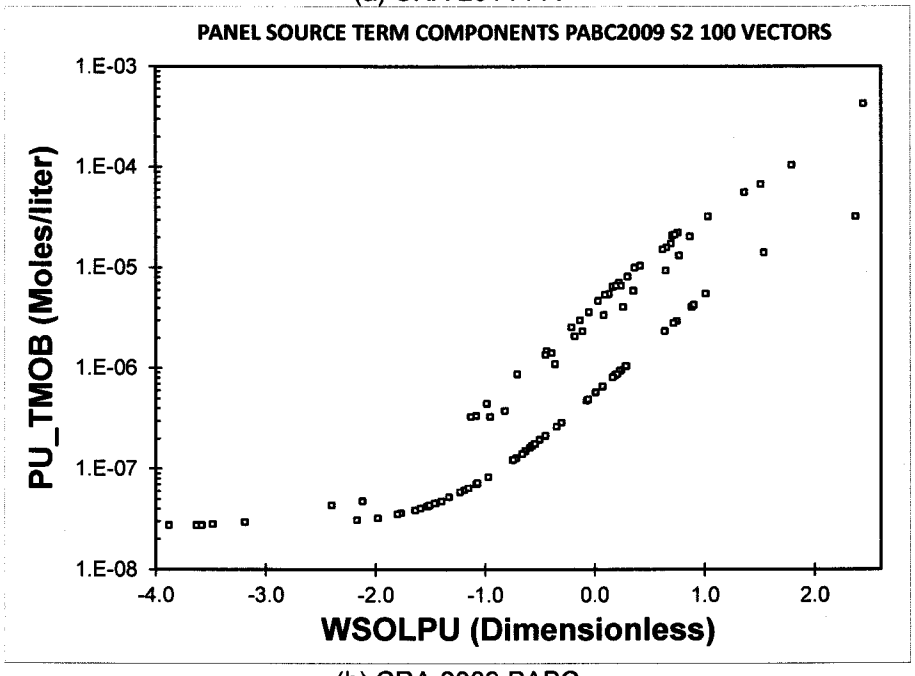


(b) CRA-2009 PABC

Figure 24. Scatter Plot of Mobilization Potential for Mineral Fragments for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.



(a) CRA-2014 PA



(b) CRA-2009 PABC

Figure 25. Scatter Plot of Total Potential Mobilized Pu in Castile Brine. Part (a) shows results from the CRA-2014 PA, where BV*k* represents *k* times of minimum brine volume (BV). Part (b) shows results from the CRA-2009 PABC.

5.2 RADIONUCLIDE DECAY

PANEL was run in the DECAY mode with the entire WIPP inventory so that plots can be generated to show how the radionuclide inventory changes over the 10,000-year regulatory period. Figures 26 to 31 show the results of these decay calculations. Figures 26 through 31 are simple x-y plots with both the CRA-2014 PA results (Part (a) in each figure) and the CRA-2009 PABC results (Part (b) in each figure) presented. Each x-y plot shows an isotopic component as the dependent variable (ordinate) in EPA Units and the time as the independent variable (abscissa). Table 14 provides definitions for the variables plotted in Figures 26 through 31.

Table 14. Definitions of Variables Plotted in Figures 26 through 31

Name	Type/Units	Description
SDETOTAL	EPA Units	Total Activity
SDEPU239	EPA Units	Activity of PU239
SDEPU240	EPA Units	Activity of PU240
SDEPU242	EPA Units	Activity of PU242
SDEAM241	EPA Units	Activity of AM241
SDEPU238	EPA Units	Activity of PU238
SDEU233	EPA Units	Activity of U233
SDEU234	EPA Units	Activity of U234
SDEU238	EPA Units	Activity of U238
SDEU236	EPA Units	Activity of U236
SDEU235	EPA Units	Activity of U235
SDETH229	EPA Units	Activity of TH229
SDETH230	EPA Units	Activity of TH230
SDENP237	EPA Units	Activity of NP237
SDERA226	EPA Units	Activity of RA226
SDETH232	EPA Units	Activity of TH232
SDEAM243	EPA Units	Activity of AM243
SDECM245	EPA Units	Activity of CM245
SDECS137	EPA Units	Activity of CS137
SDESR90	EPA Units	Activity of SR90
SDEPB210	EPA Units	Activity of PB210
SDEPA231	EPA Units	Activity of PA231
SDECM248	EPA Units	Activity of CM248
SDEPU244	EPA Units	Activity of PU244
SDECM243	EPA Units	Activity of CM243
SDERA228	EPA Units	Activity of RA228
SDEPU241	EPA Units	Activity of PU241
SDECM244	EPA Units	Activity of CM244
SDECF252	EPA Units	Activity of CF252
LDETOTAL	EPA Units	Lumped Activity of TOTAL
LDEPU239	EPA Units	Lumped Activity of PU239
LDETH230	EPA Units	Lumped Activity of TH230
LDEU234	EPA Units	Lumped Activity of U234
LDEAM241	EPA Units	Lumped Activity of AM241
LDEPU238	EPA Units	Lumped Activity of PU238

Figure 26 shows the decay behavior for the Am and Pu isotopes over time. In general, the Pu isotopic inventory is steady over time with the exception of Pu238 which decays away by about 3000 years. In addition, Am241 decays away over time with the final inventory of Am241 at 10,000 years about 10^{-6} of the initial inventory. Comparison of total inventory (SDETOTAL) between both the CRA-2014 PA and CRA-2009 PABC indicates that there are some relatively

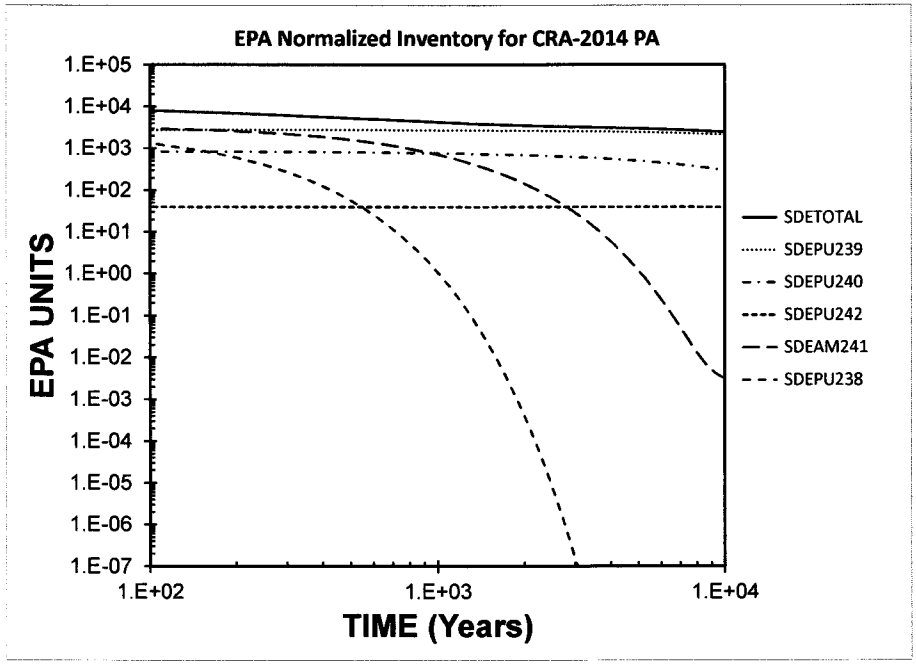
large differences in inventory. The inventory of both the CRA-2014 PA and CRA-2009 PABC start at a similar level, but the CRA-2014 inventory is about 1.45% higher. The CRA-2014 inventory remains higher throughout the 10,000 year regulatory period. The CRA-2014 inventory in EPA Units is about 44.58% higher at 10,000 years after decommissioning than the CRA-2009 PABC inventory.

Figure 27 shows the decay behavior of the U isotopes over time. The U isotopes for the CRA-2014 PA are fairly steady over time with U234 and U236 isotopes increasing over time due to PU238 decay to U234 (half-life = 87.74 years) and PU240 decay to U236 (half-life = 6537 years). For the CRA-2009 PABC it was estimated that U234 and U236 isotopes increase over time. The U235 inventory increases during 10,000 years about 0.024 EPA units for the CRA-2014 PA and 0.017 EPA units for the CRA-2009 PABC. Use of log scale for EPA Unit in Figure 27 and a nearly 20 times higher inventory at start makes the U235 inventory seem to remain steady over time.

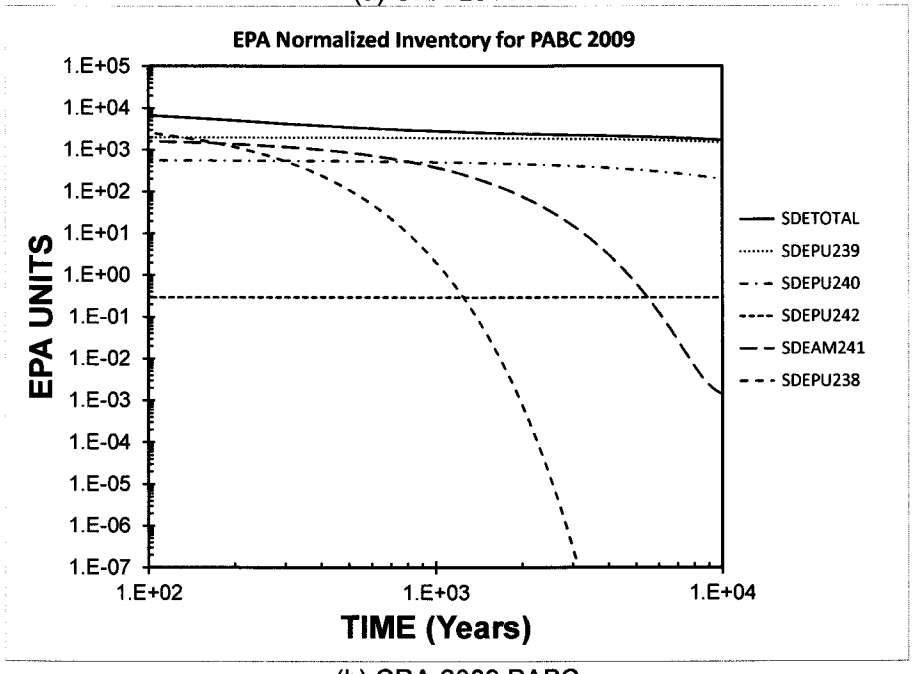
Figures 28 and 30 show the decay behaviors for isotopes TH229, TH230, TH232, NP237, RA226, RA228 AM243, PB210, PA231, PU241, PU244, CF252, CM243, CM244, CM248 and CM245. In Figure 30 the inventories of isotopes RA228, PU241, CM244, and CF252, with much less than 1.0 x 10-12 EPA units, are not shown. Isotopes AM243, CM243, and CM245 that are located on top of decay chain (used in one of PANEL code, **PANEL_SUBRS.FOR**, in CMS library **LIBPANEL**), decrease their inventory throughout 10,000 year period (Figure 28 and Figure 30). Isotopes TH229, PB210, and PA231 that are located at the bottom of the decay chain, increase their inventories (Figure 28 and Figure 30). However, isotopes TH230, TH232, NP237, RA226, PU244, and CM248 are located in the middle of a decay chain such that inventory changes of each isotope depend on its half-life and its parent isotope's half-life. Figure 28 shows that the inventory of each isotope consequently increases, exhibits a minimum, or decreases over time.

Figure 29 shows the decay behavior for the fission products: SR90 and CS137. Both of these isotopes decay away before 2000 years.

The time dependent behavior of the lumped radionuclides (Figure 31) is directly attributable to the component radionuclides in the lumped radionuclides. Therefore, the AM241L behavior is like that of AM241 (Figure 26). The PU239L behavior is like that of PU239 (Figure 26). The U234L behavior is like that of U234 (Figure 27). The PU238L behavior is like that of PU238 (Figure 26). The TH230L behavior is like that of TH230 (Figure 28).

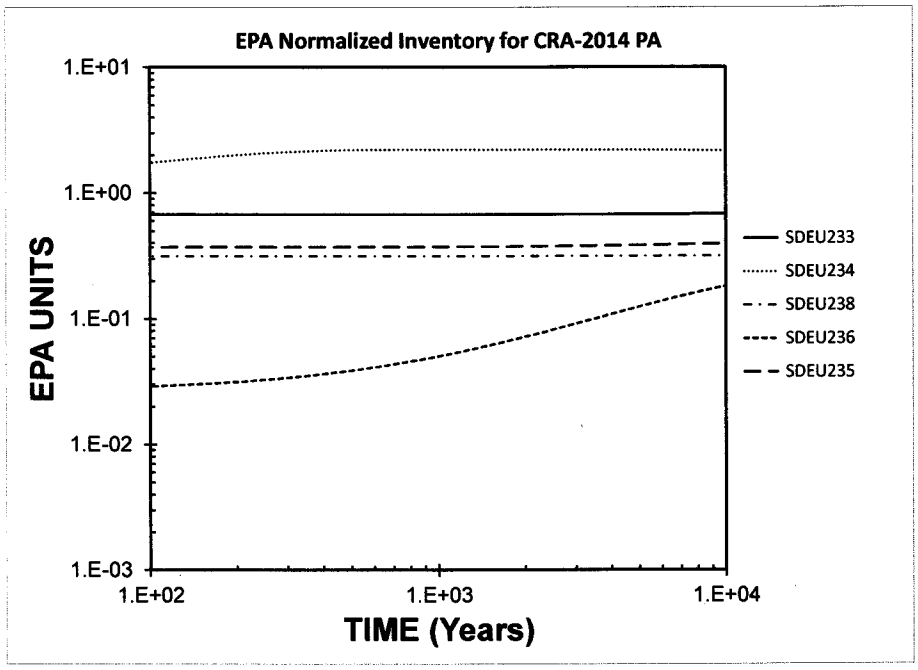


(a) CRA-2014 PA

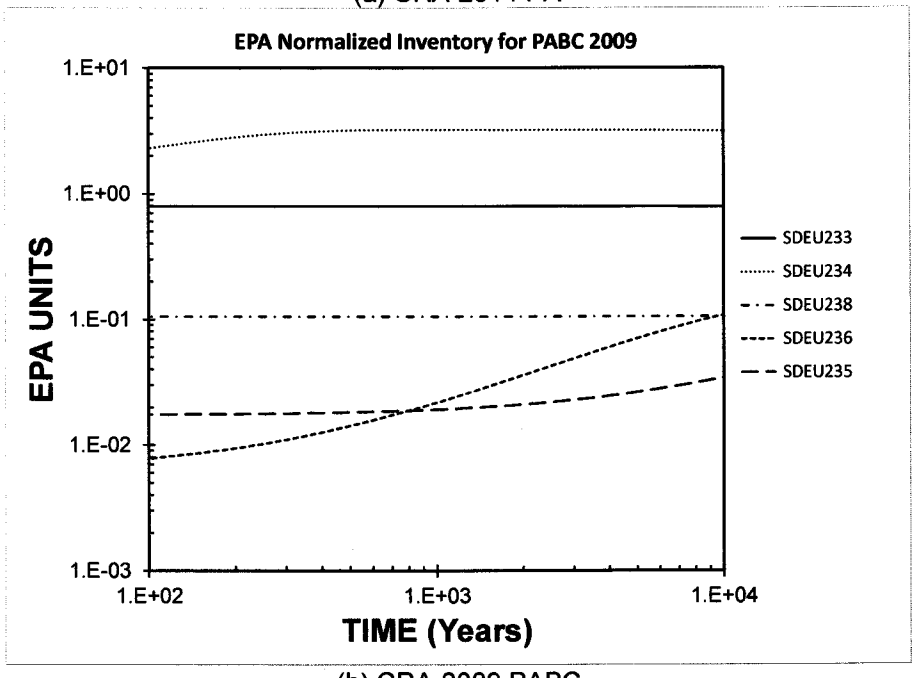


(b) CRA-2009 PABC

Figure 26. Time dependent inventories of Am and Pu isotopes. Part (a) shows results from the CRA-2014 PA. Part (b) shows results from the CRA-2009 PABC.

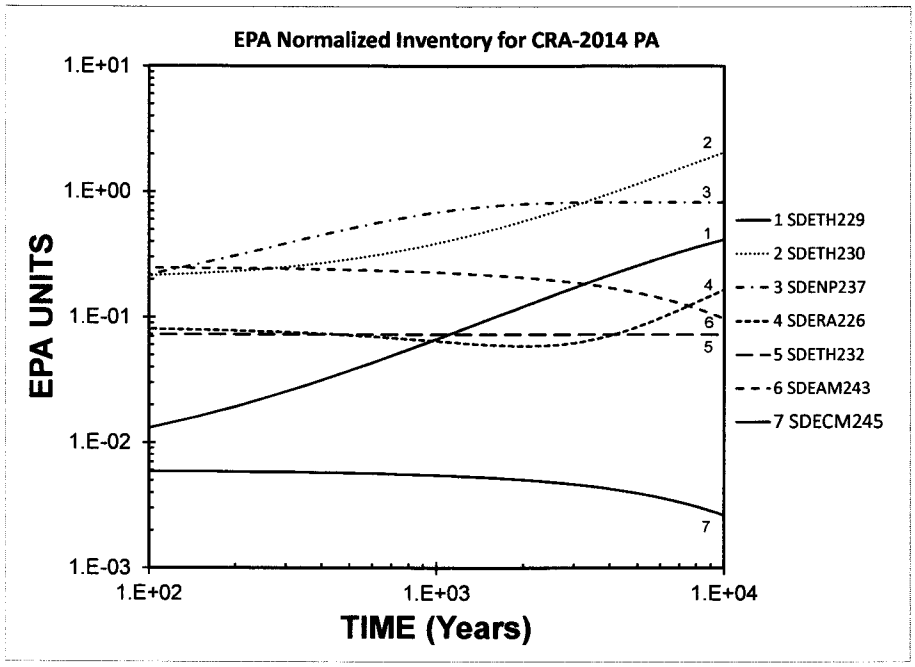


(a) CRA-2014 PA

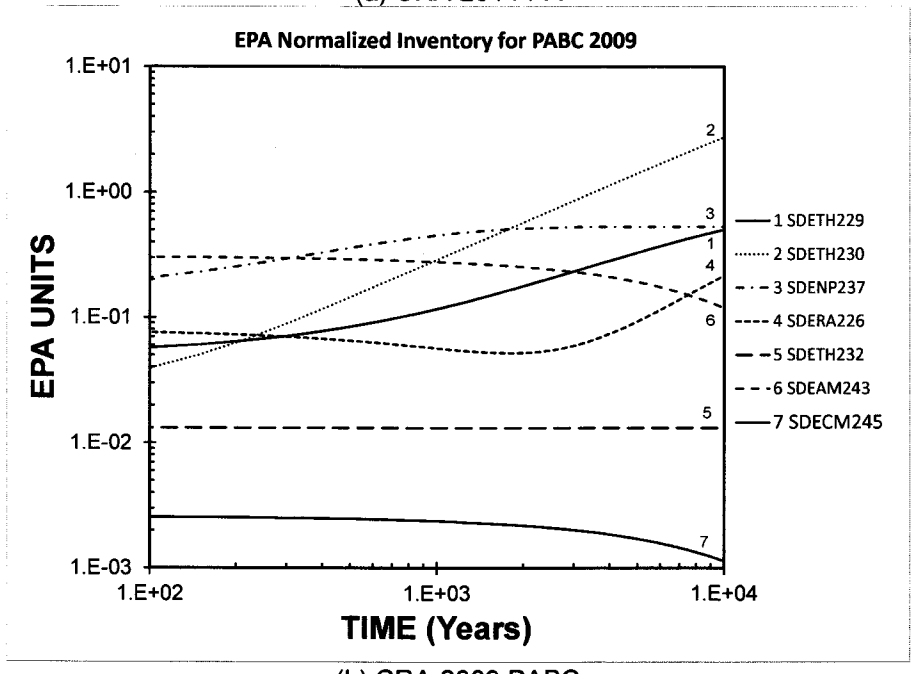


(b) CRA-2009 PABC

Figure 27. Time dependent inventories of U isotopes. Part (a) shows results from the CRA-2014 PA. Part (b) shows results from the CRA-2009 PABC.

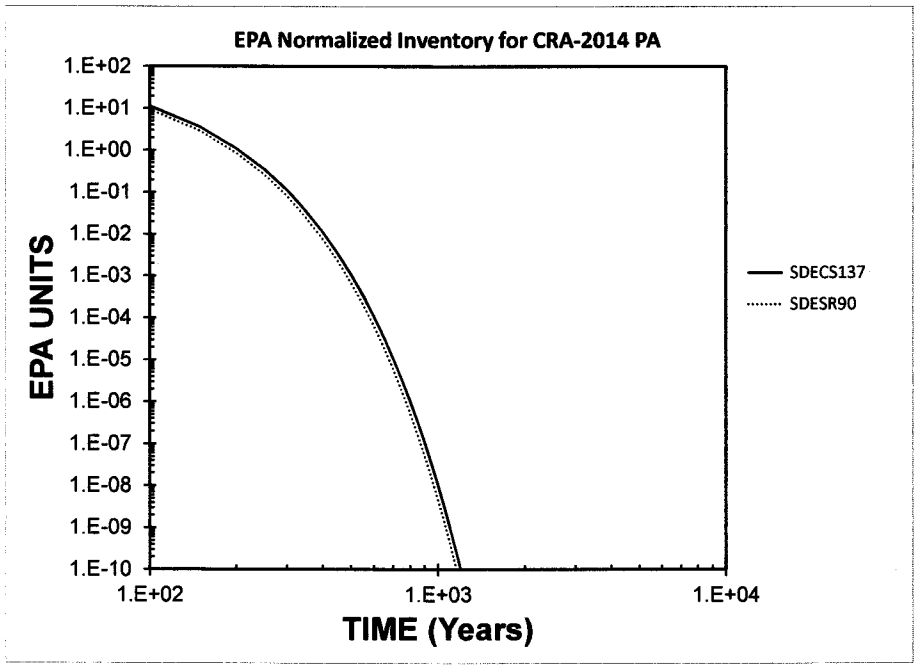


(a) CRA-2014 PA

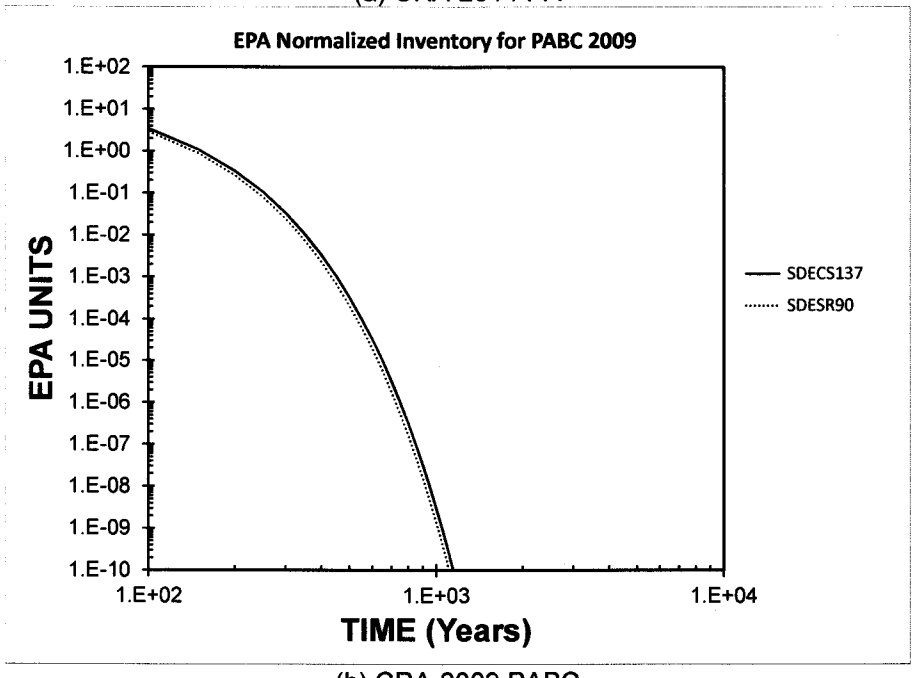


(b) CRA-2009 PABC

Figure 28. Time dependent inventories of various isotopes. Part (a) shows results from the CRA-2014 PA. Part (b) shows results from the CRA-2009 PABC.

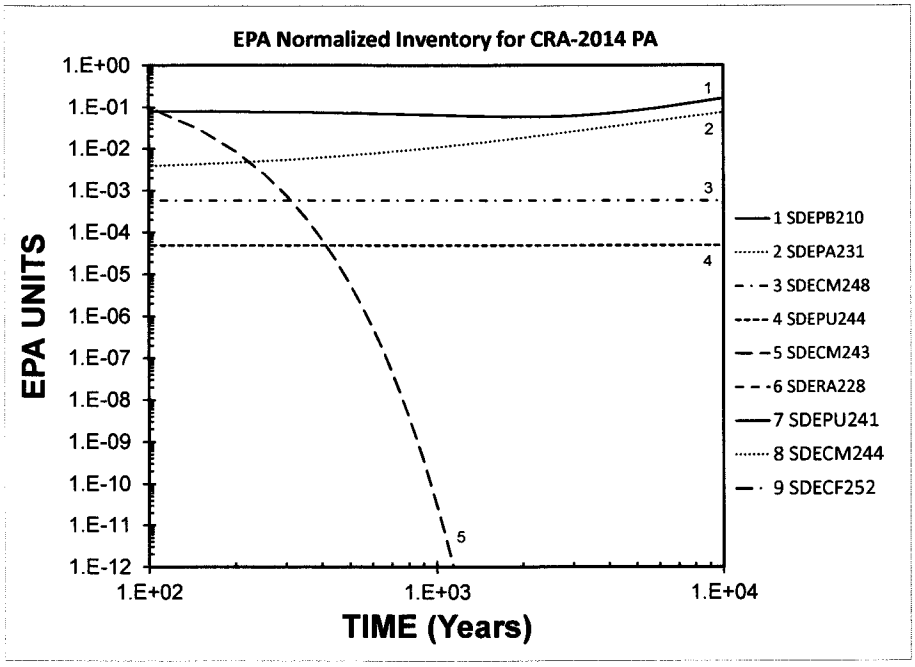


(a) CRA-2014 PA

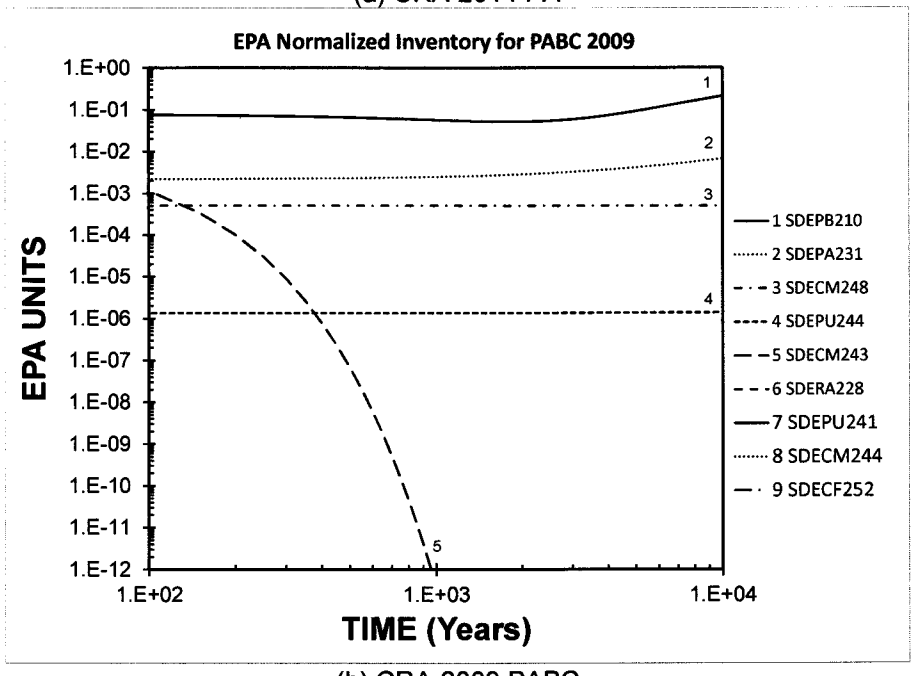


(b) CRA-2009 PABC

Figure 29. Time dependent inventories of Sr and Cs isotopes. Part (a) shows results from the CRA-2014 PA. Part (b) shows results from the CRA-2009 PABC.

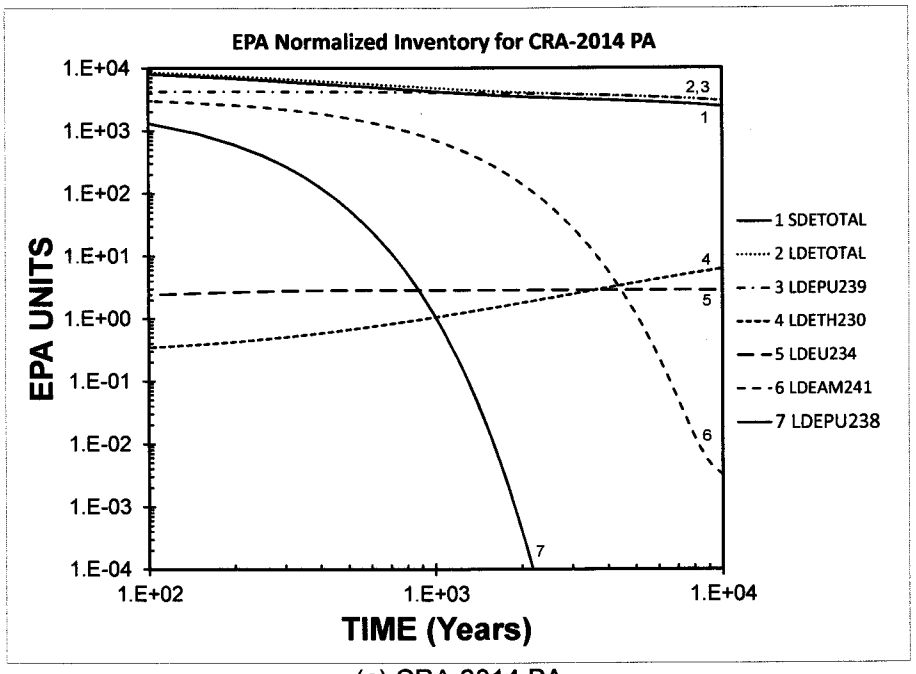


(a) CRA-2014 PA

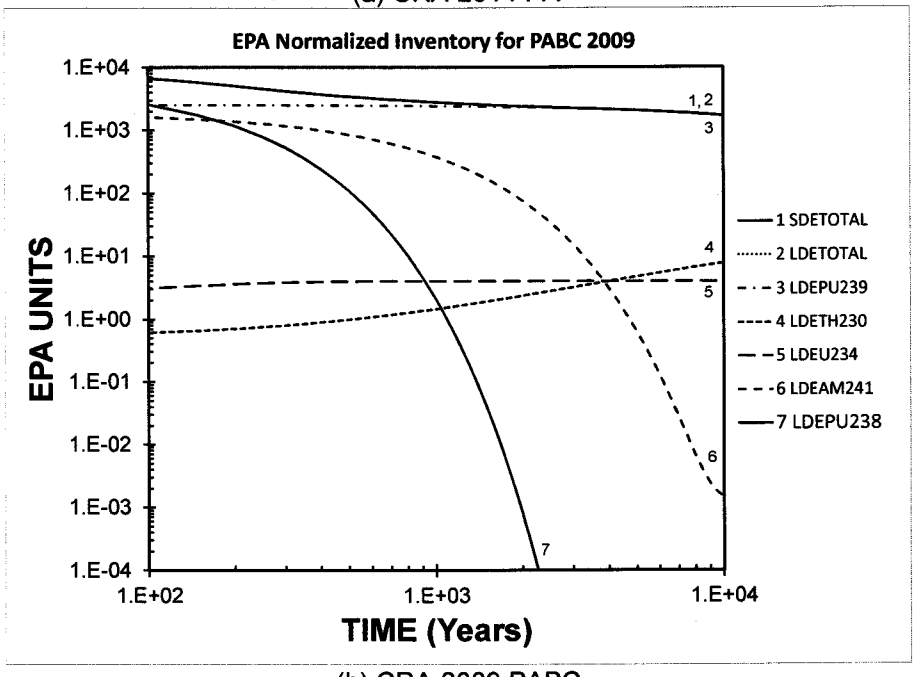


(b) CRA-2009 PABC

Figure 30. Time dependent inventories of various minor isotopes. Part (a) shows results from the CRA-2014 PA. Part (b) shows results from the CRA-2009 PABC.



(a) CRA-2014 PA



(b) CRA-2009 PABC

Figure 31. Time dependent inventories of lumped isotopes. Part (a) shows results from the CRA-2014 PA. Part (b) shows results from the CRA-2009 PABC.

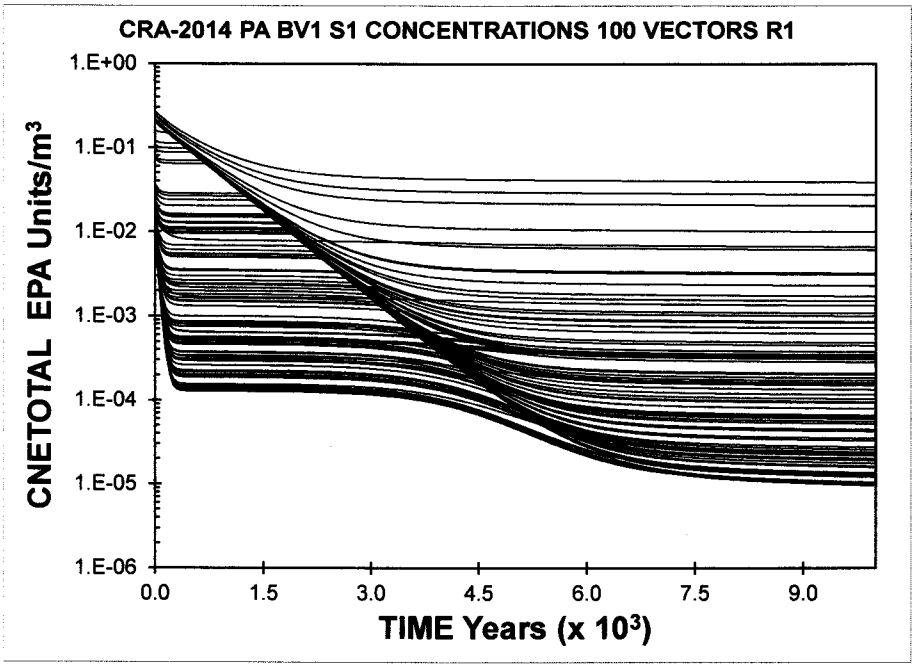
5.3 PANEL CONCENTRATIONS

PANEL concentration results are presented in Figures 32 through 41. Figures 32 through 41 are horsetail plots. "Horsetail" plots show values of individual variables for all vectors in a scenario as a function of time for the entire 10,000-year regulatory compliance period. These plots are an effective method for demonstrating the potential range and behavior of results. Thus, the independent variable (abscissa) in Figures 32 through 41 is time in years. The dependent variable (ordinate) in Figures 32 through 41 is concentration in EPA units per cubic meter. Part (a) – (e) shows results from the CRA-2014 PA with BVk (k = 1, 2, 3, 4, 5). Part (f) shows results from the CRA-2009 PABC.

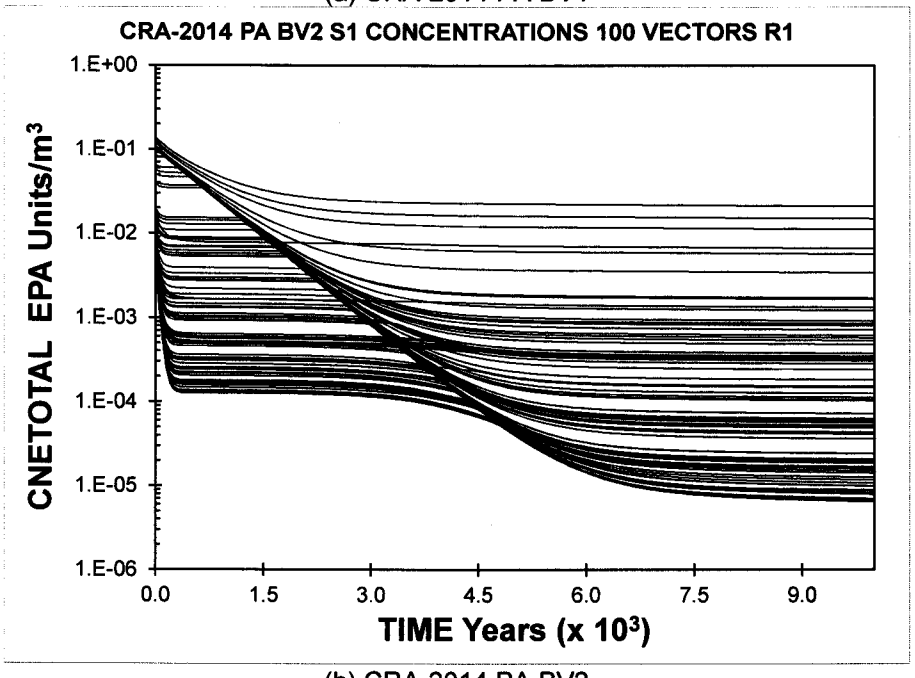
Figure 32 shows the total mobilized concentration (summed for the individual radionuclides from Table 11) in Salado brine in EPA units per cubic meter. Figure 37 shows the total mobilized concentration in Castile brine in EPA units per cubic meter. These concentration values are supplied to CCDFGF to calculate DBR releases. Figures 33, 34, 35, and 36 show the mobilized concentrations for the lumped radionuclides in Salado brine. Figures 38, 39, 40, and 41 show the mobilized concentrations for the lumped radionuclides in Castile brine.

At early times (before 2000 years), the total mobilized concentrations (in both Salado and Castile brines) have their highest values because of the contribution of AM (see Figures 33 and 38). After about 4000 years, the contribution from AM decreases because of the decay of AM241. After about 4000 years, the total mobilized concentrations are dominated by PU (see Figures 34 and 39). U and TH contributions are orders of magnitudes lower than PU (see Figures 35, 36, 40 and 41).

The CRA-2014 PA results for total mobilized concentrations show similar variability (comparable spread in the curves) to those seen in the CRA-2009 PABC results. Total mobilized concentration values for the CRA-2014 PA decreases slightly as the brine volume increases. Total mobilized concentrations with BV3, BV4 and BV5 brine volumes show nearly comparable variability and value range. The CRA-2014 PA results with BV1 for total mobilized concentrations are comparable variability and value range to seen in the CRA-2009 PABC, though the solubility of the +III and +IV oxidation states is increased (Table 1). Slight solubility changes seem to rarely affect total mobilized concentrations.

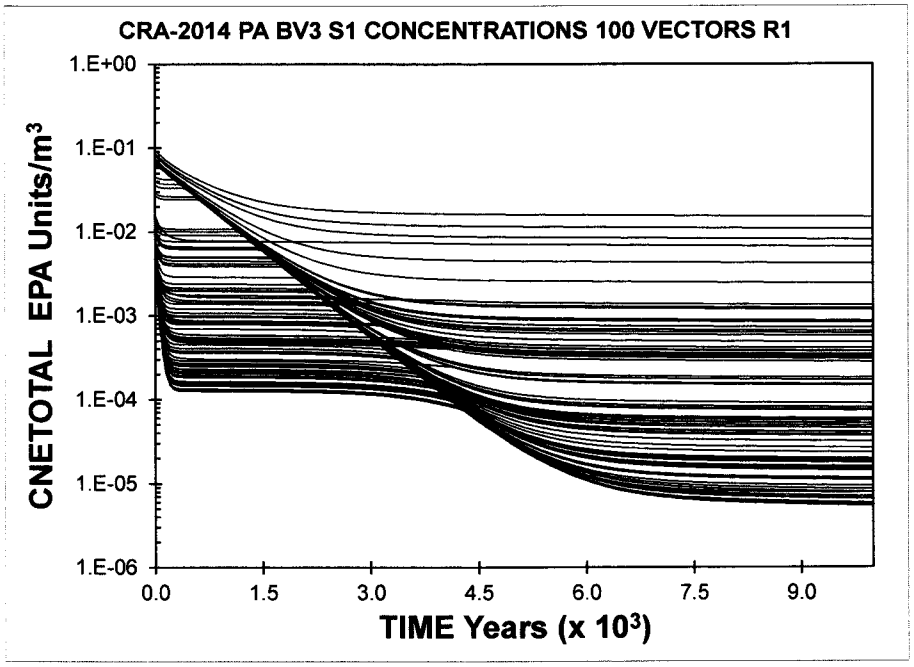


(a) CRA-2014 PA BV1

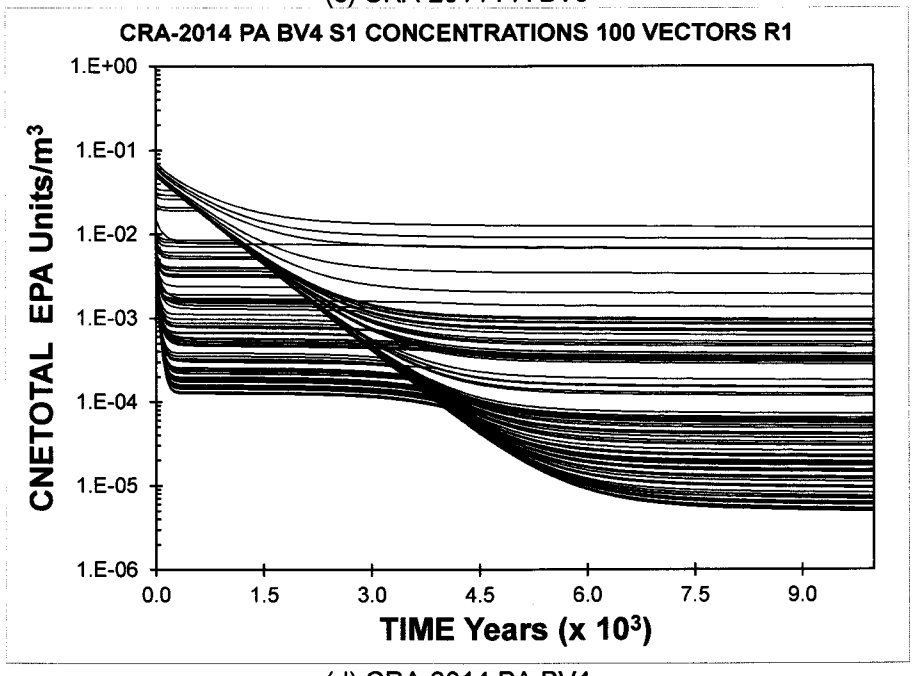


(b) CRA-2014 PA BV2

Figure 32. Time dependent total concentrations in Salado brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

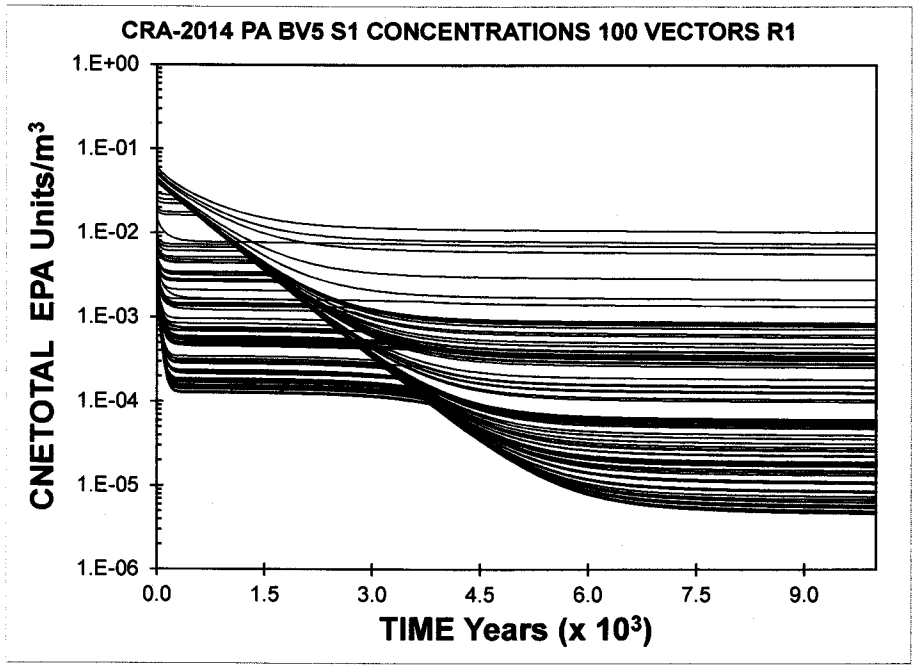


(c) CRA-2014 PA BV3

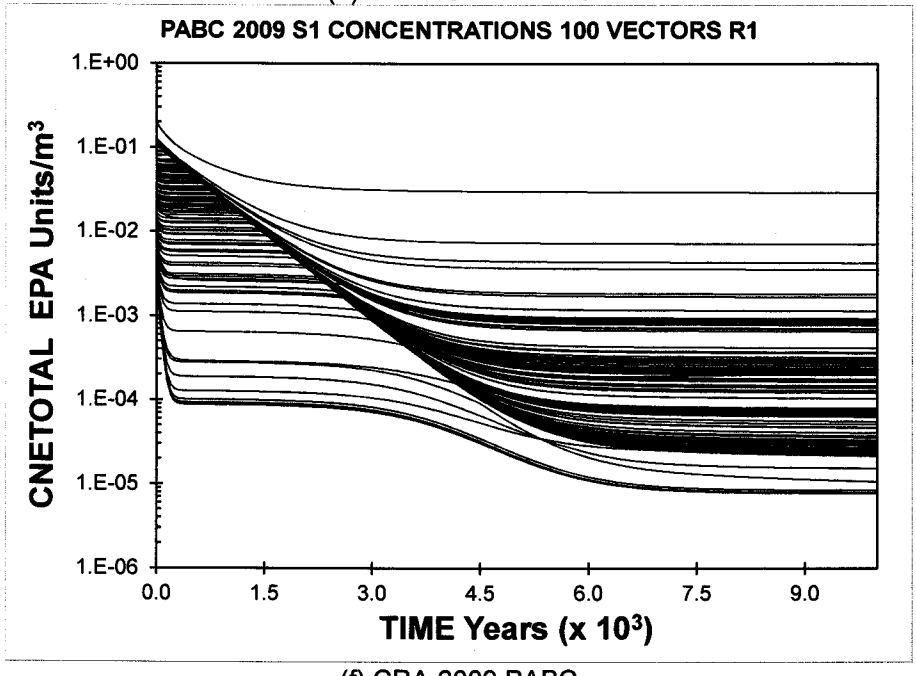


(d) CRA-2014 PA BV4

Figure 33 (*continued*). Time dependent total concentrations in Salado brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

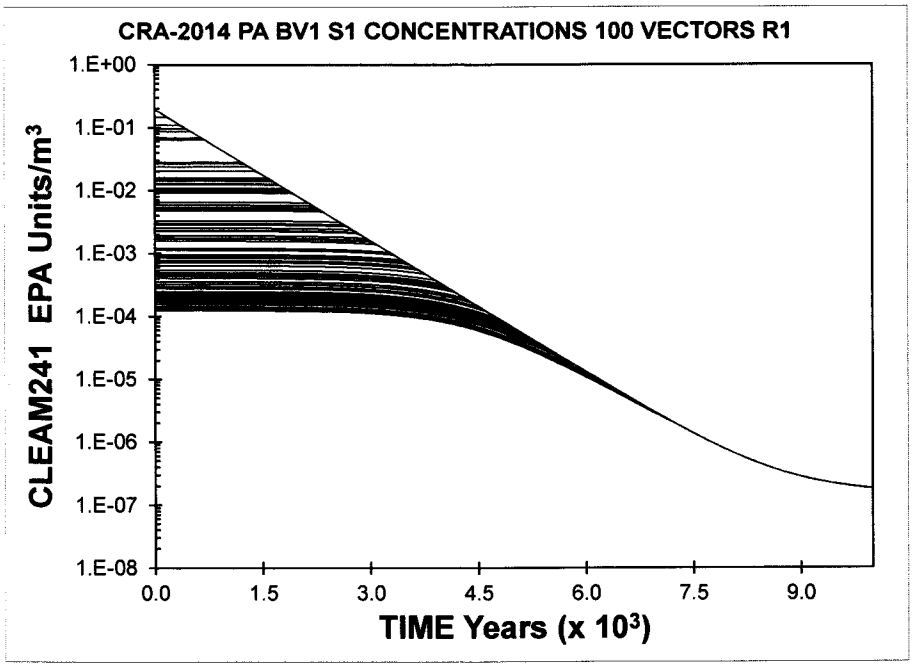


(e) CRA-2014 PA BV5

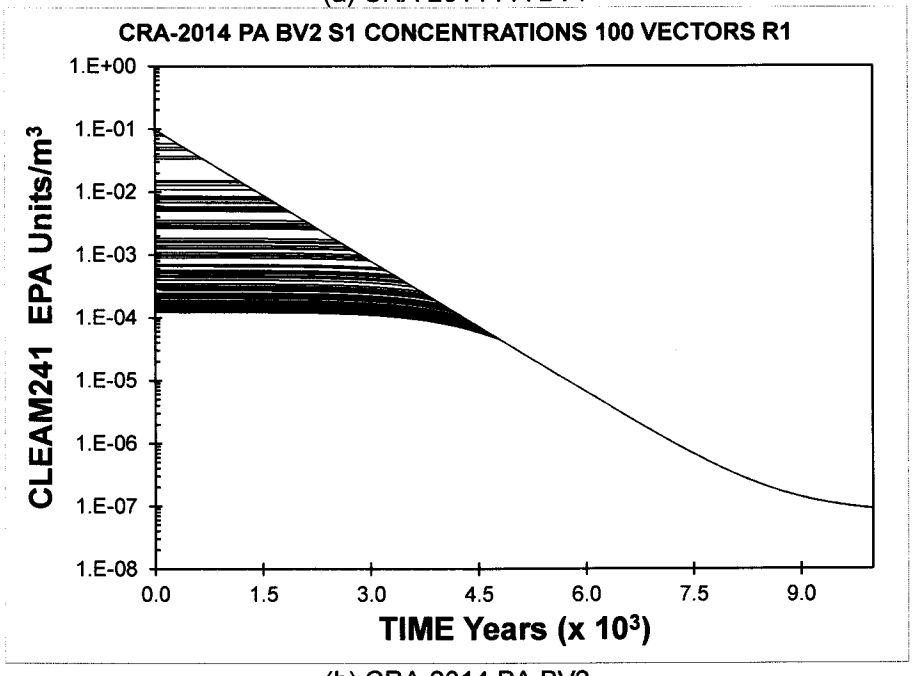


(f) CRA-2009 PABC

Figure 34 (*continued*). Time dependent total concentrations in Salado brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

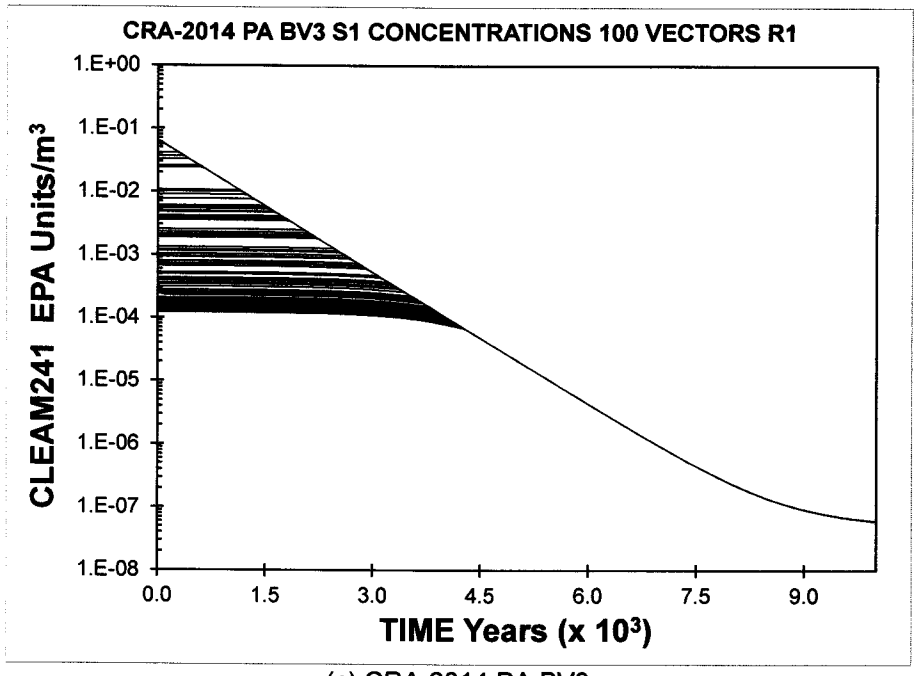


(a) CRA-2014 PA BV1

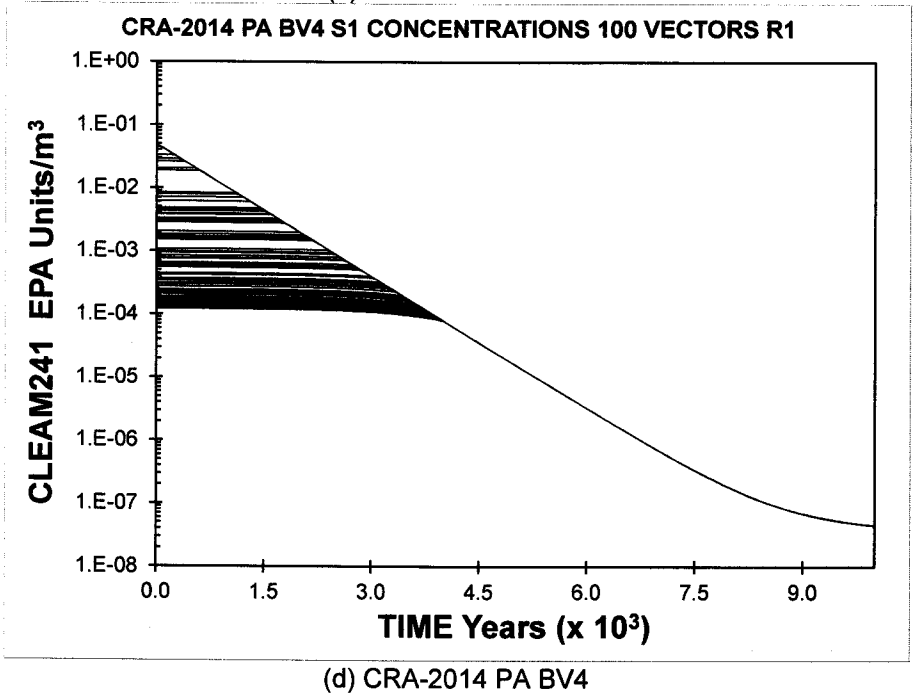


(b) CRA-2014 PA BV2

Figure 35. Time dependent AM241L concentration in Salado brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

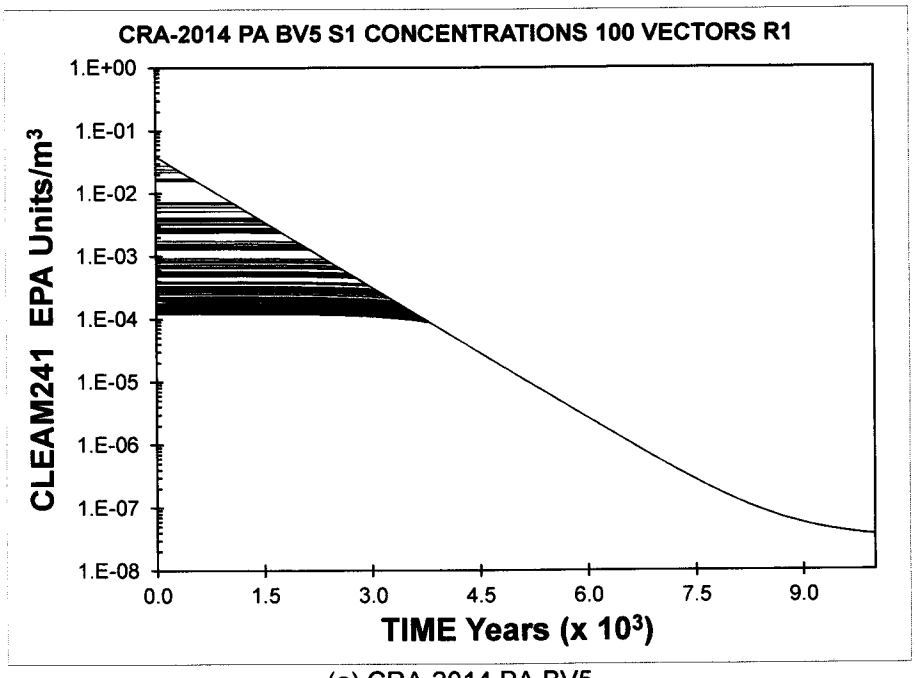


(c) CRA-2014 PA BV3

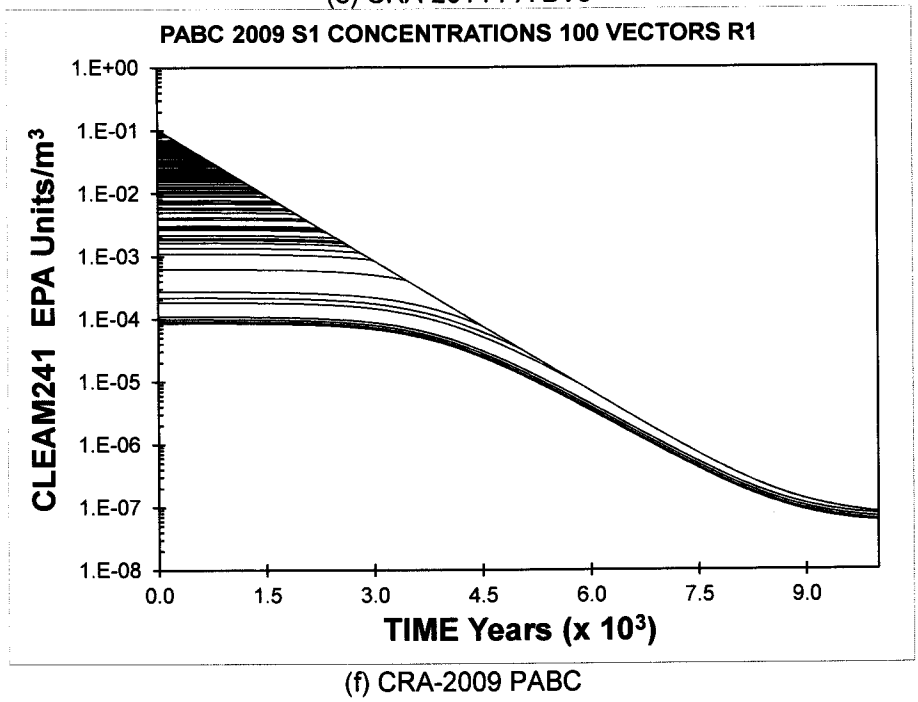


(d) CRA-2014 PA BV4

Figure 36 (*continued*). Time dependent AM241L concentration in Salado brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

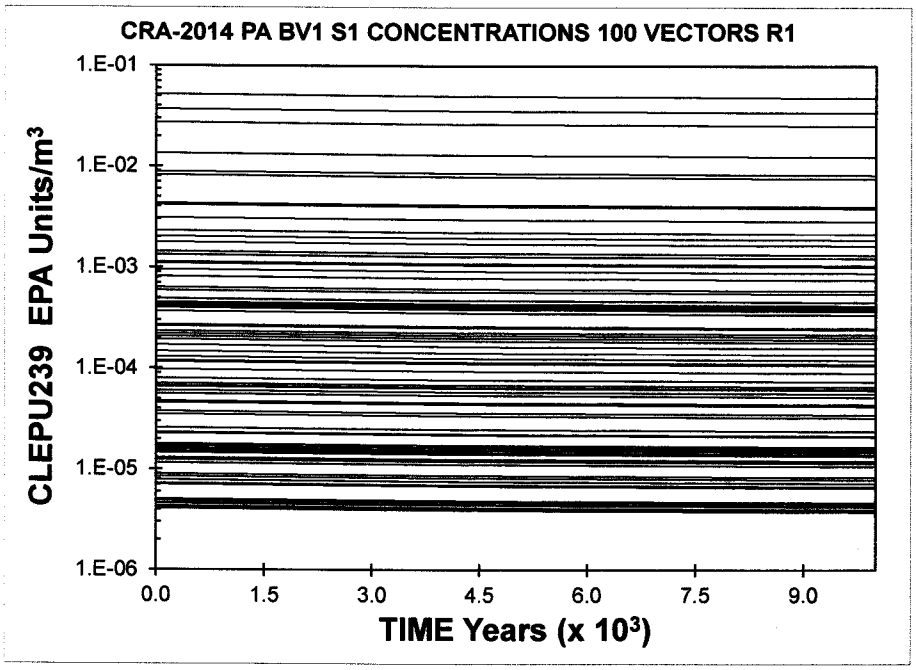


(e) CRA-2014 PA BV5

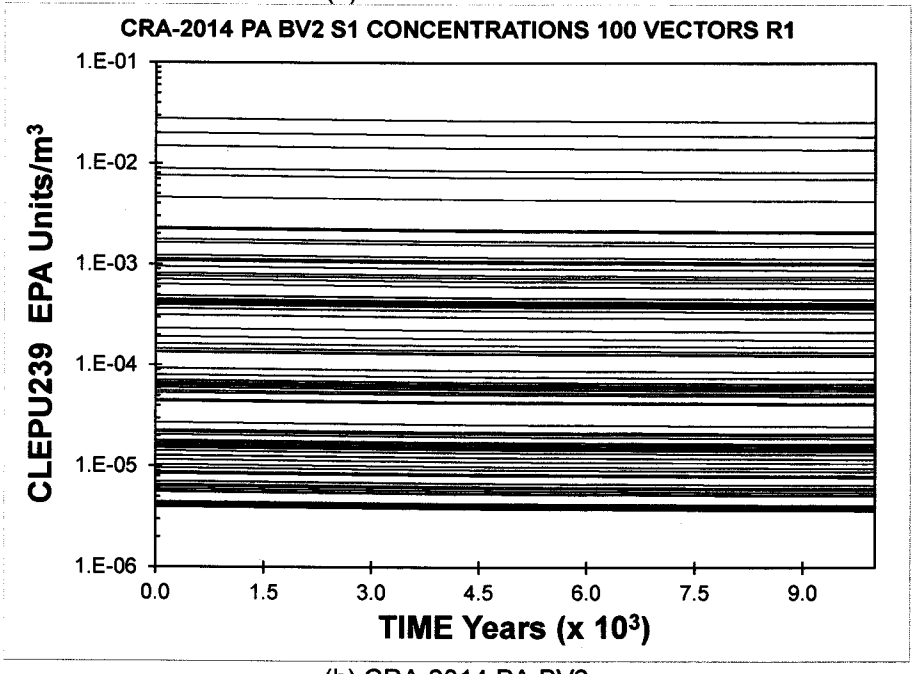


(f) CRA-2009 PABC

Figure 37 (*continued*). Time dependent AM241L concentration in Salado brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

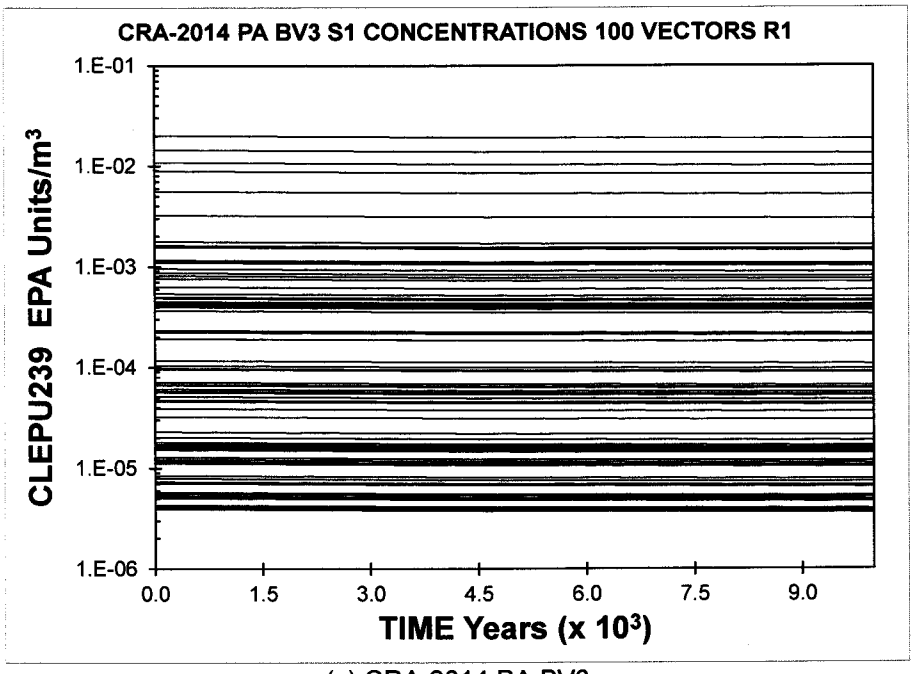


(a) CRA-2014 PA BV1

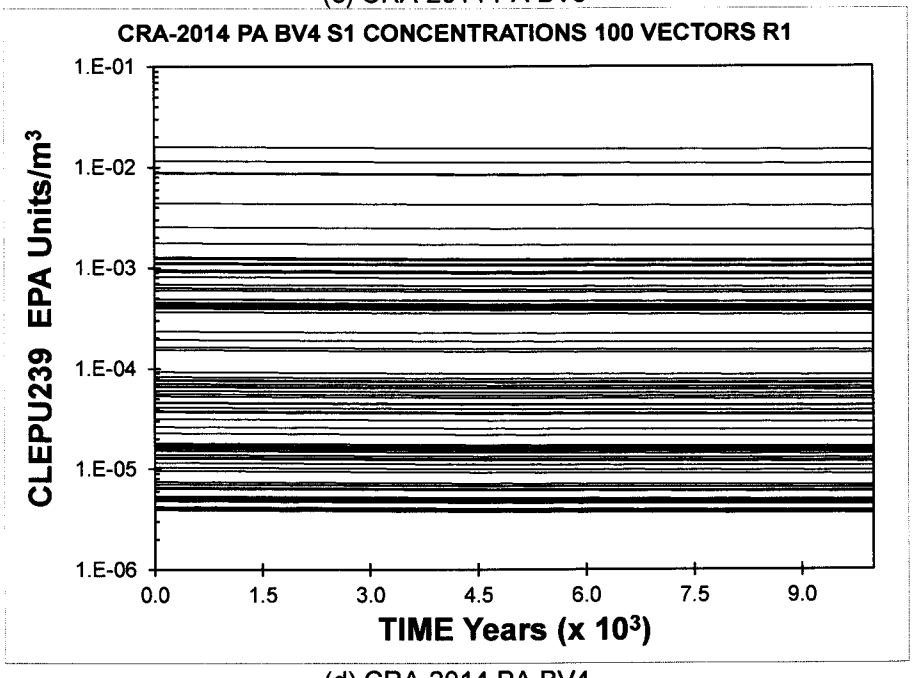


(b) CRA-2014 PA BV2

Figure 38. Time dependent PU239L concentration in Salado brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

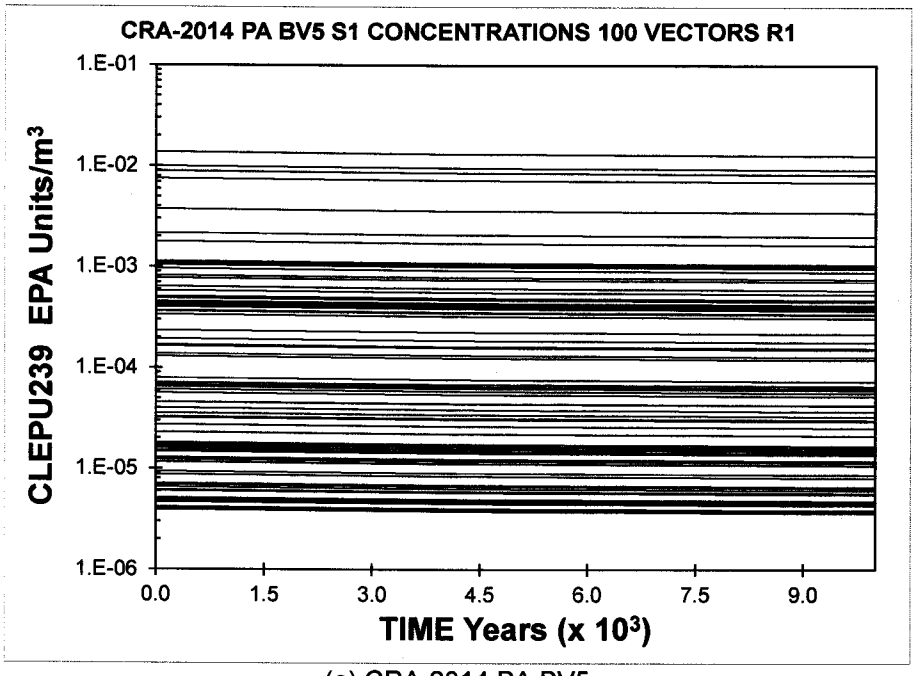


(c) CRA-2014 PA BV3

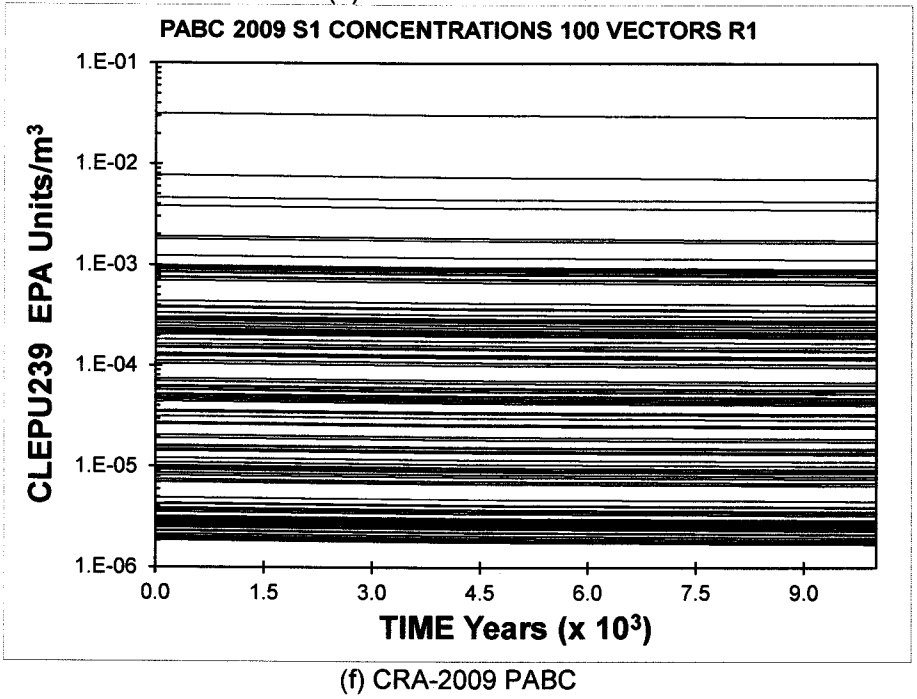


(d) CRA-2014 PA BV4

Figure 39 (*continued*). Time dependent PU239L concentration in Salado brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

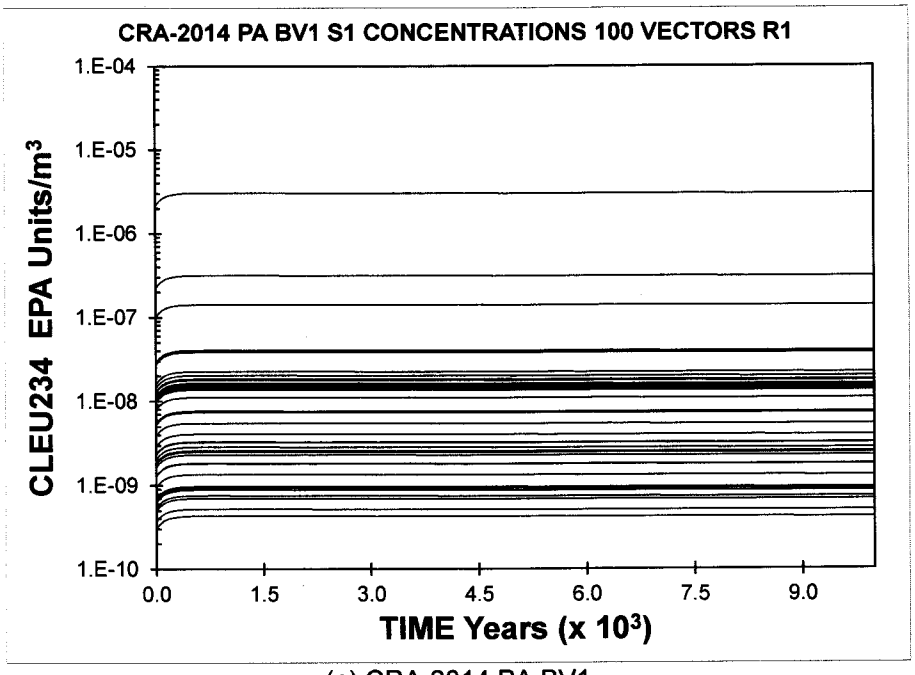


(e) CRA-2014 PA BV5

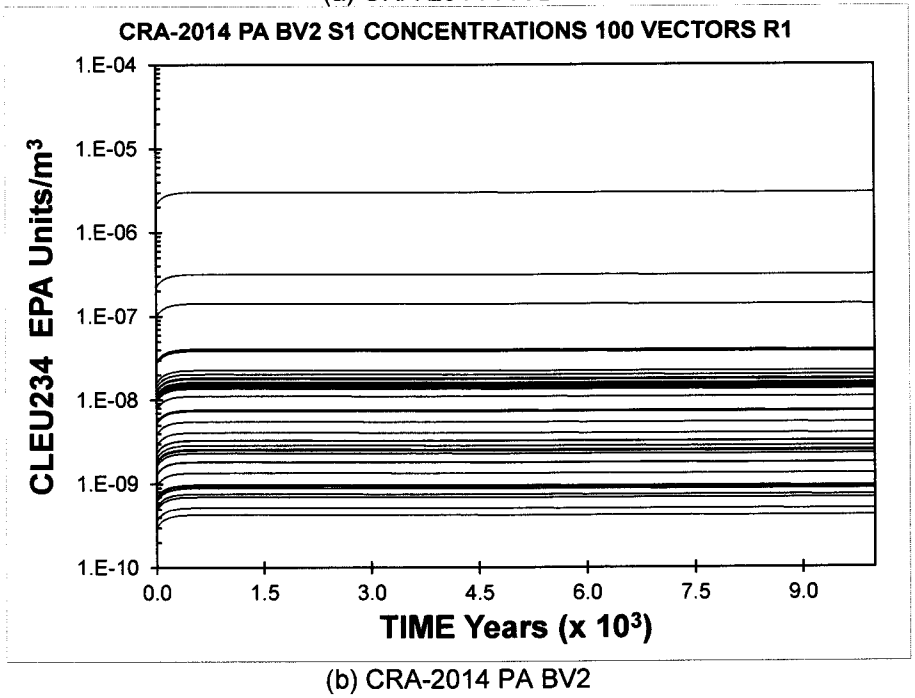


(f) CRA-2009 PABC

Figure 40 (*continued*). Time dependent PU239L concentration in Salado brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

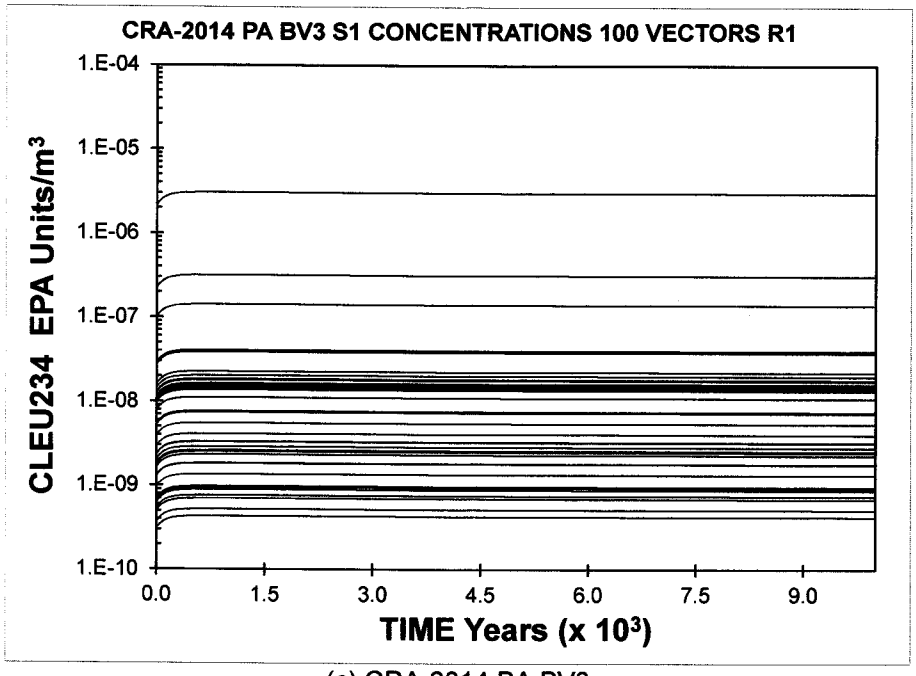


(a) CRA-2014 PA BV1

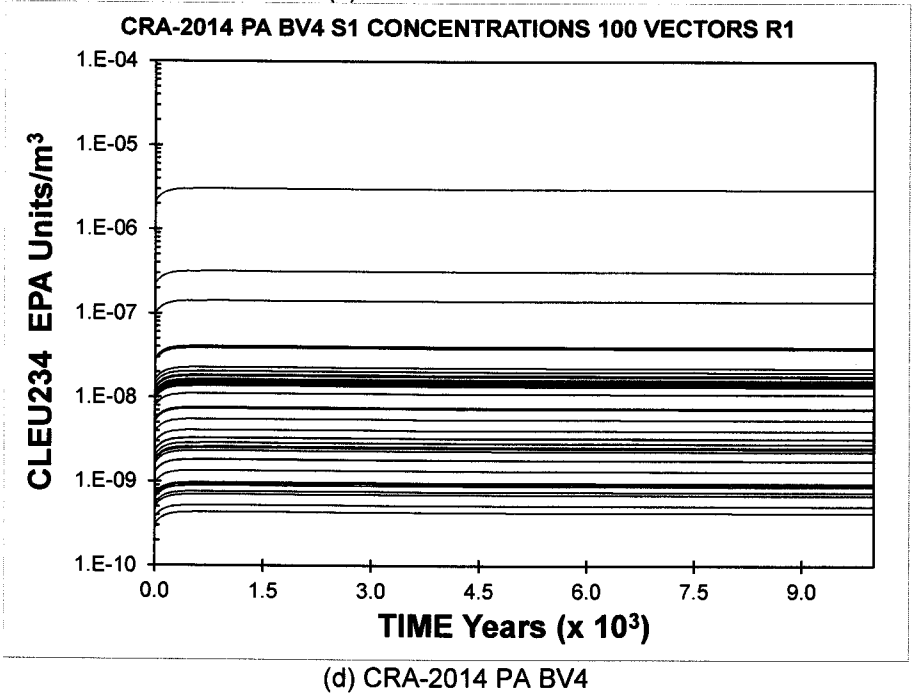


(b) CRA-2014 PA BV2

Figure 41. Time dependent U234L concentration in Salado brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

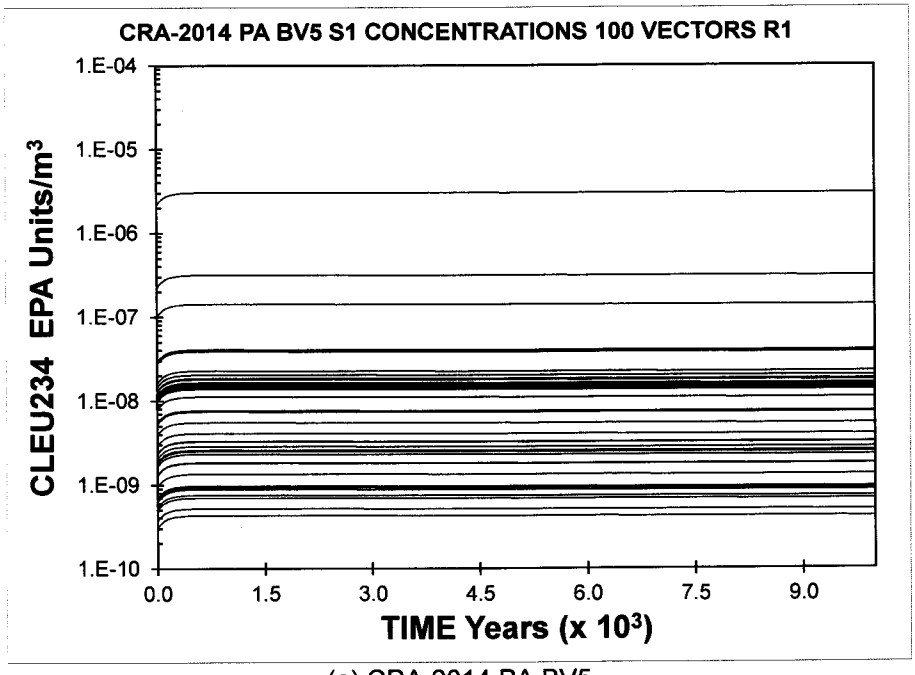


(c) CRA-2014 PA BV3

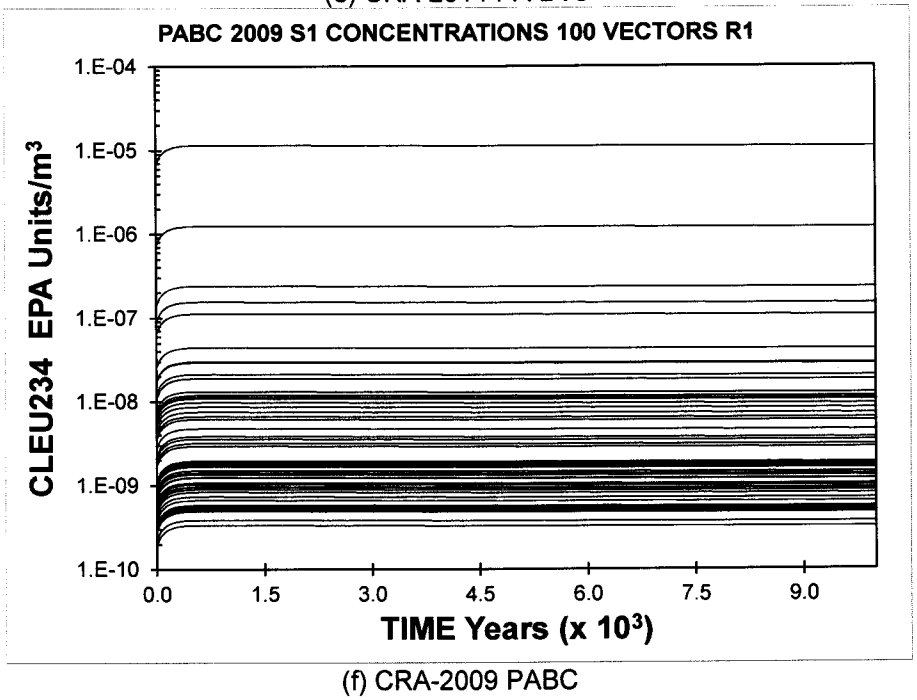


(d) CRA-2014 PA BV4

Figure 42 (*continued*). Time dependent U234L concentration in Salado brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

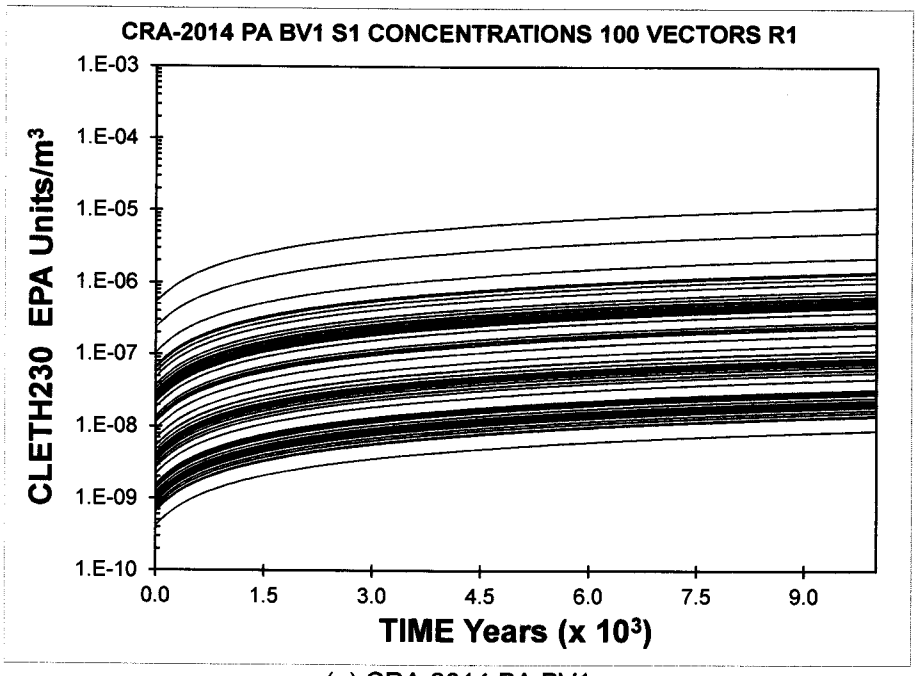


(e) CRA-2014 PA BV5

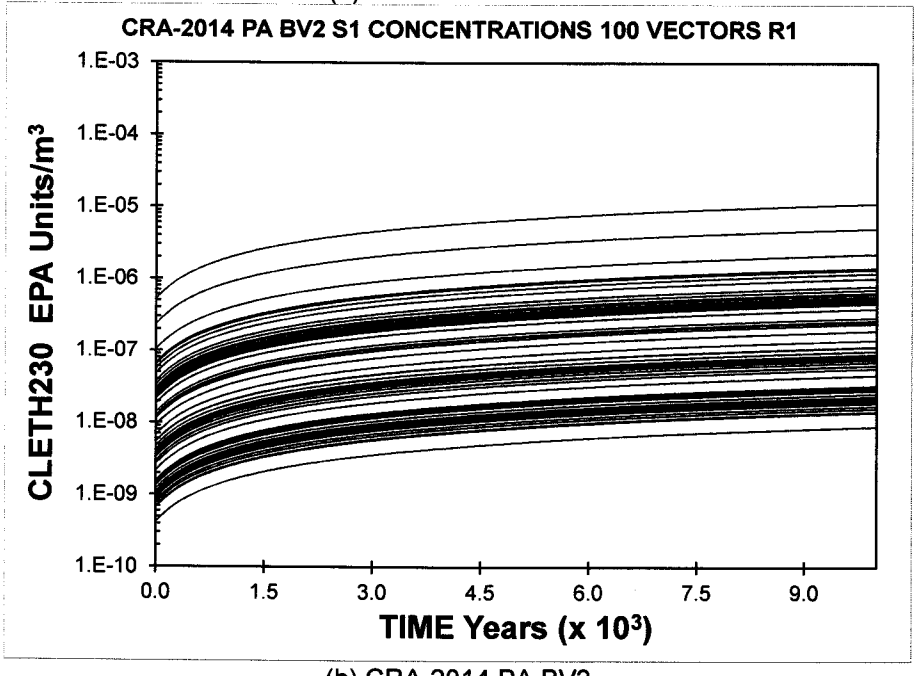


(f) CRA-2009 PABC

Figure 43 (*continued*). Time dependent U234L concentration in Salado brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

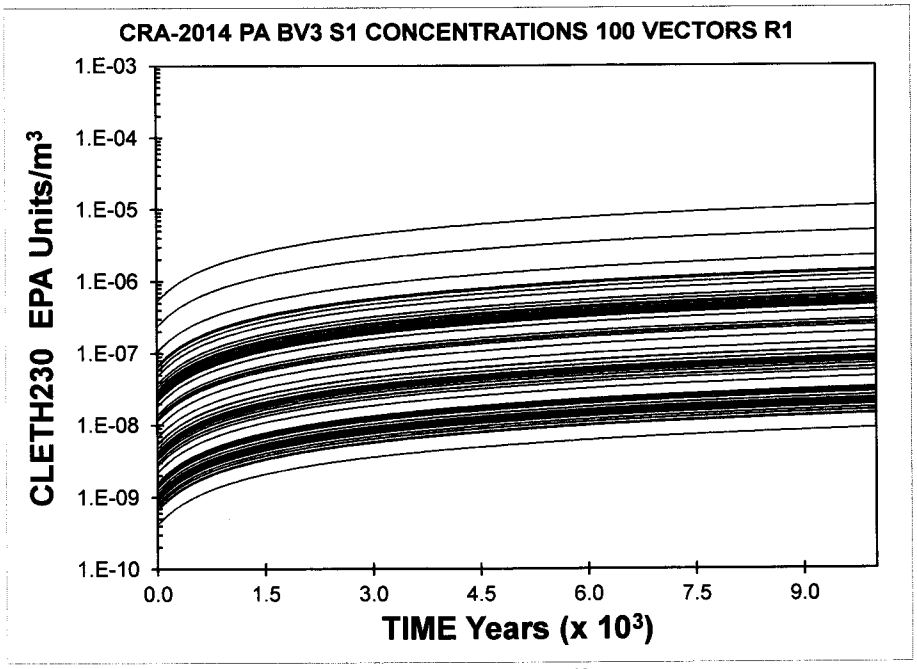


(a) CRA-2014 PA BV1

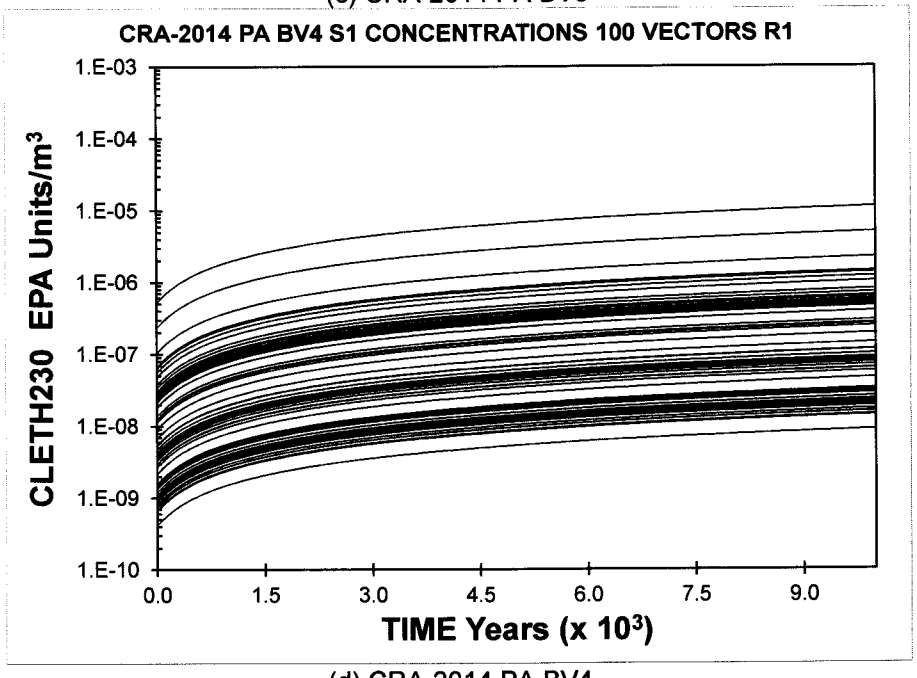


(b) CRA-2014 PA BV2

Figure 44. Time dependent TH230L concentration in Salado brine, where (a) BV1 and (b) BV1. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

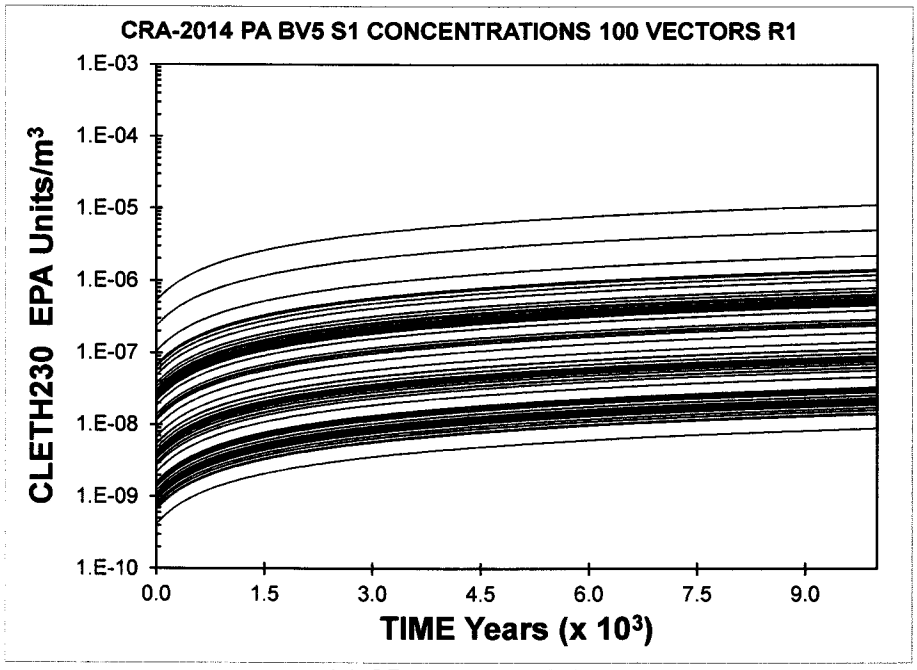


(c) CRA-2014 PA BV3

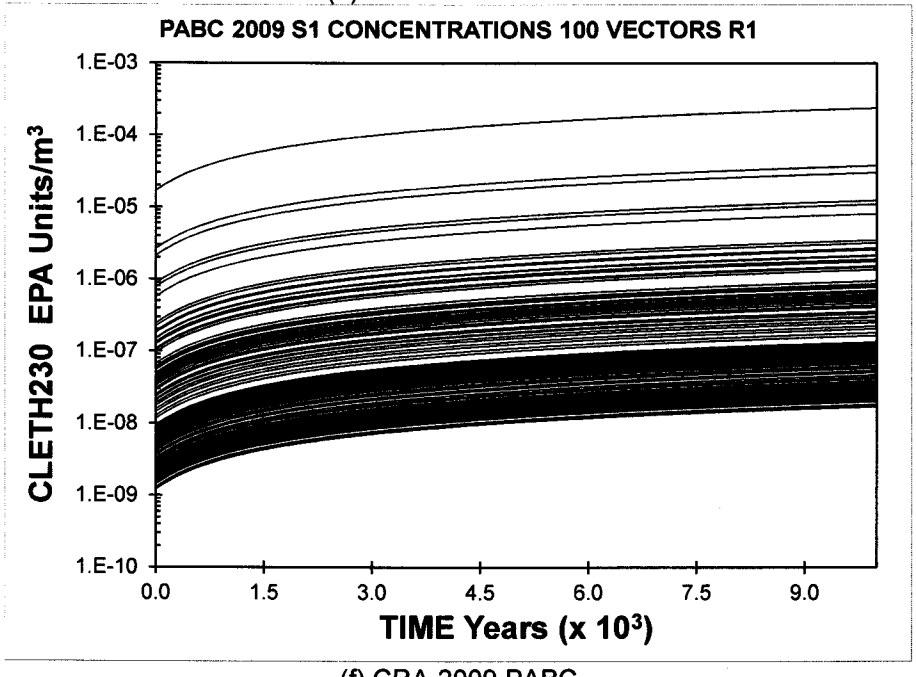


(d) CRA-2014 PA BV4

Figure 45 (*continued*). Time dependent TH230L concentration in Salado brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

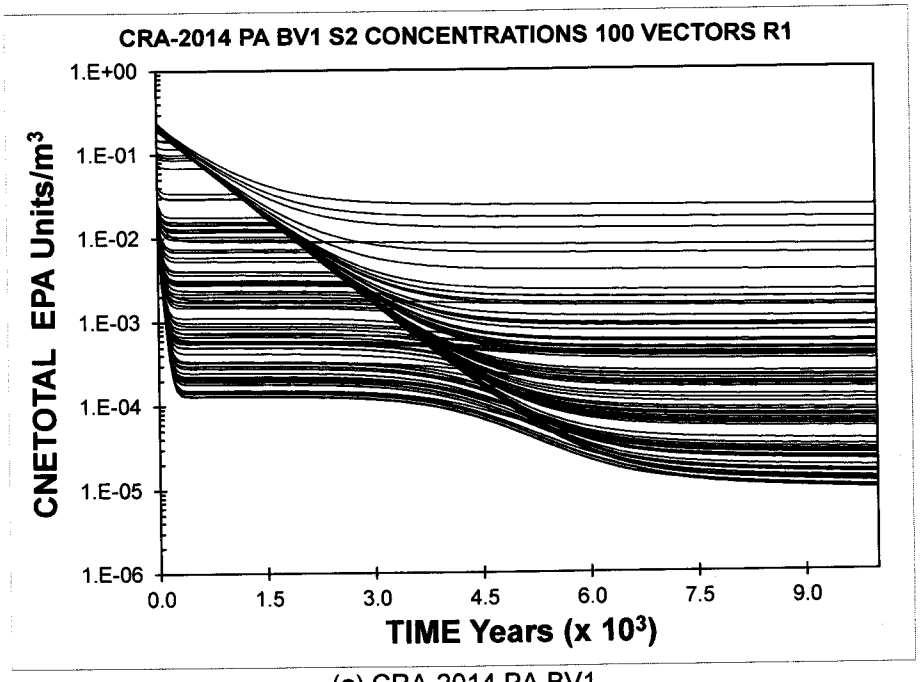


(e) CRA-2014 PA BV5

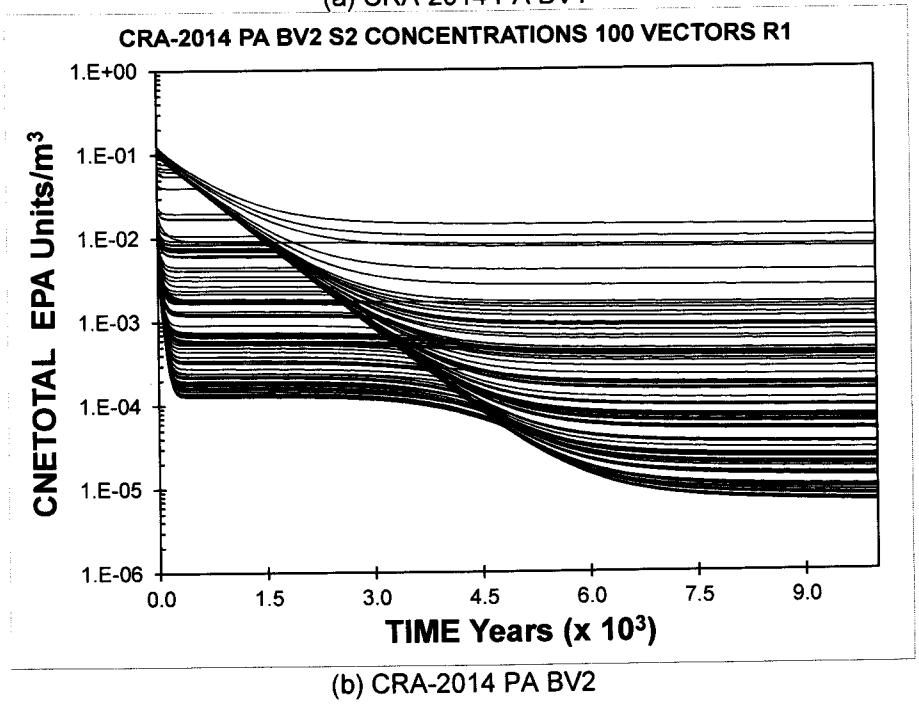


(f) CRA-2009 PABC

Figure 46 (*continued*). Time dependent TH230L concentration in Salado brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

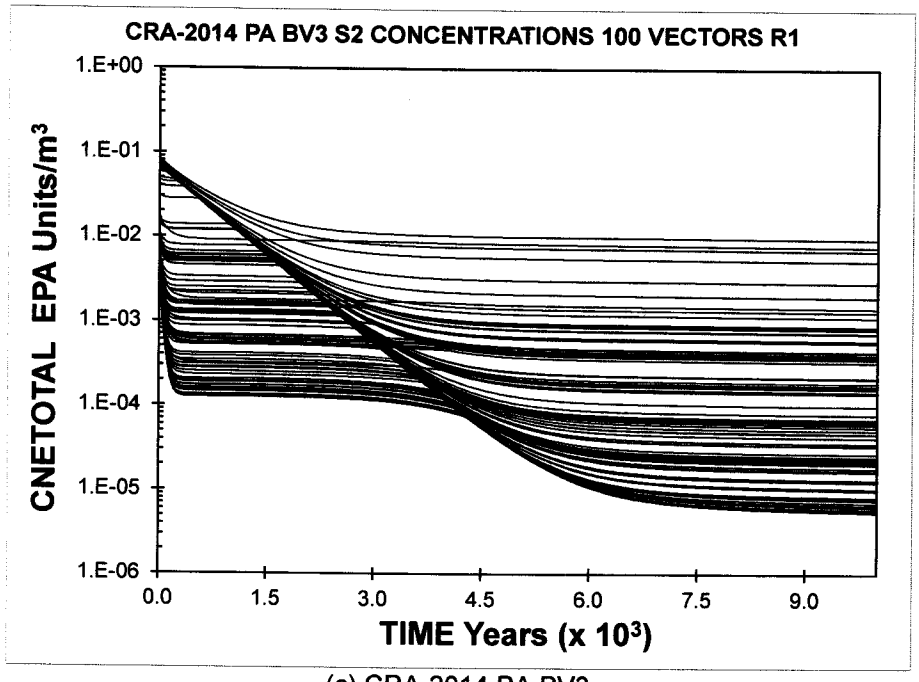


(a) CRA-2014 PA BV1

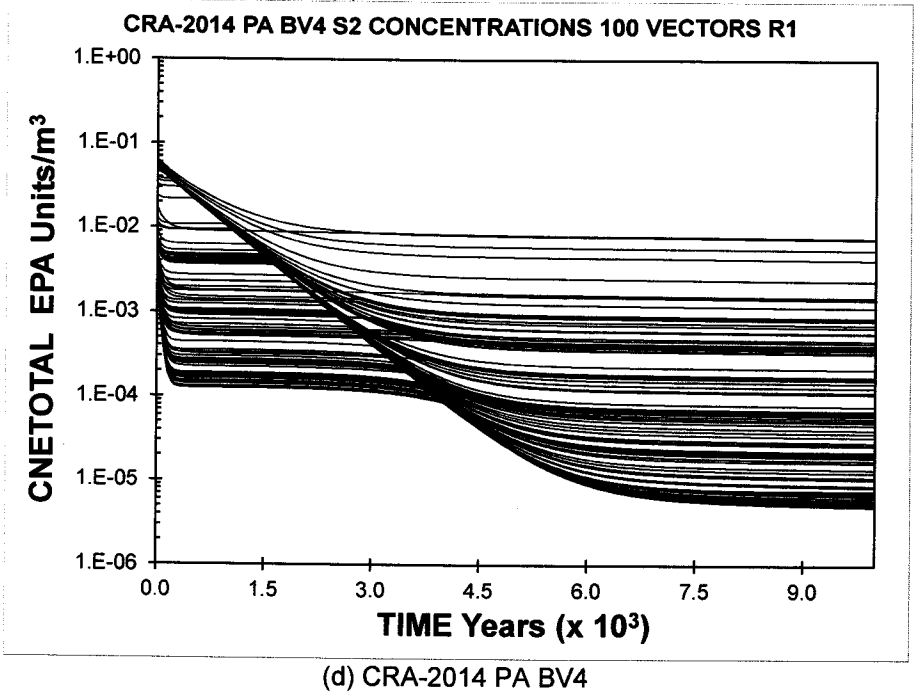


(b) CRA-2014 PA BV2

Figure 47. Time dependent total concentrations in Castile brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

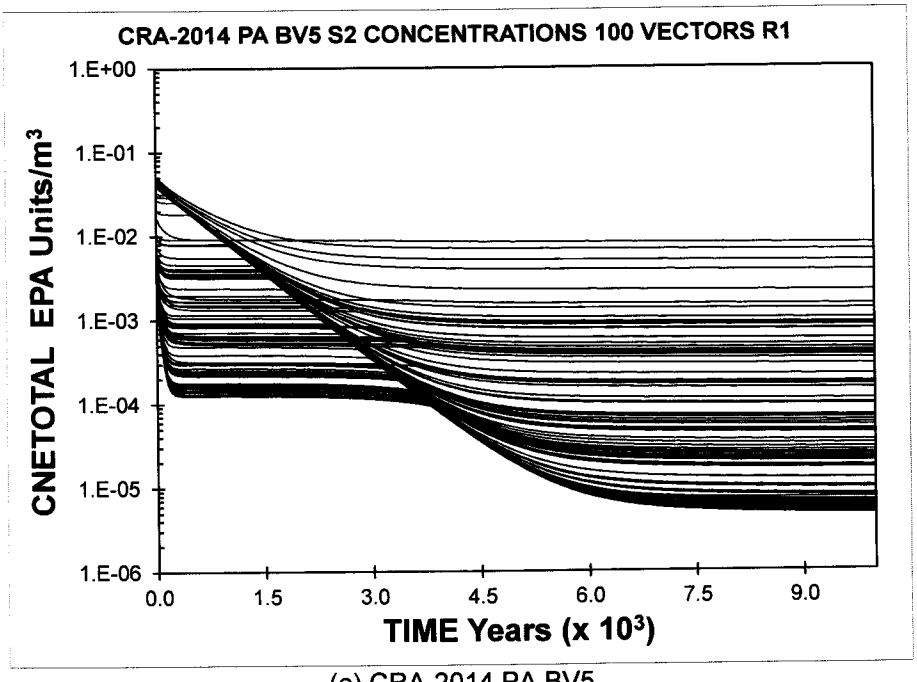


(c) CRA-2014 PA BV3

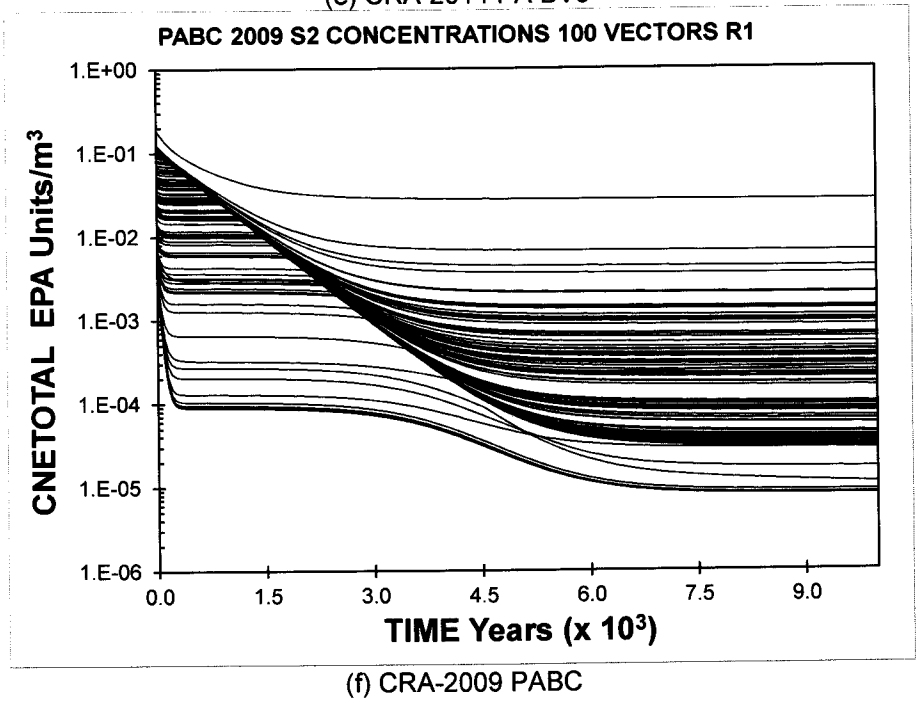


(d) CRA-2014 PA BV4

Figure 48 (*continued*). Time dependent total concentrations in Castile brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

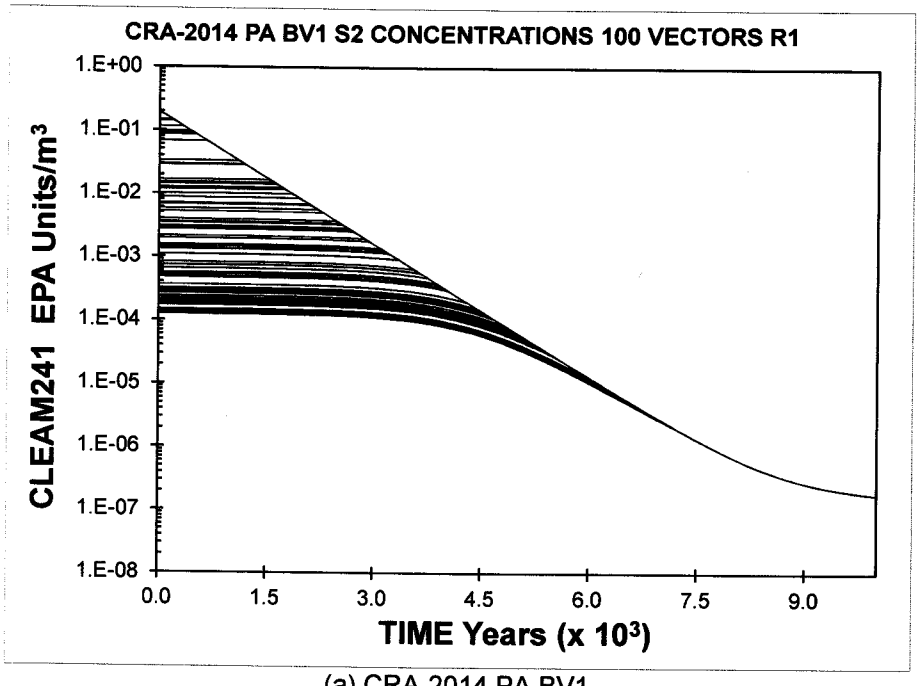


(e) CRA-2014 PA BV5

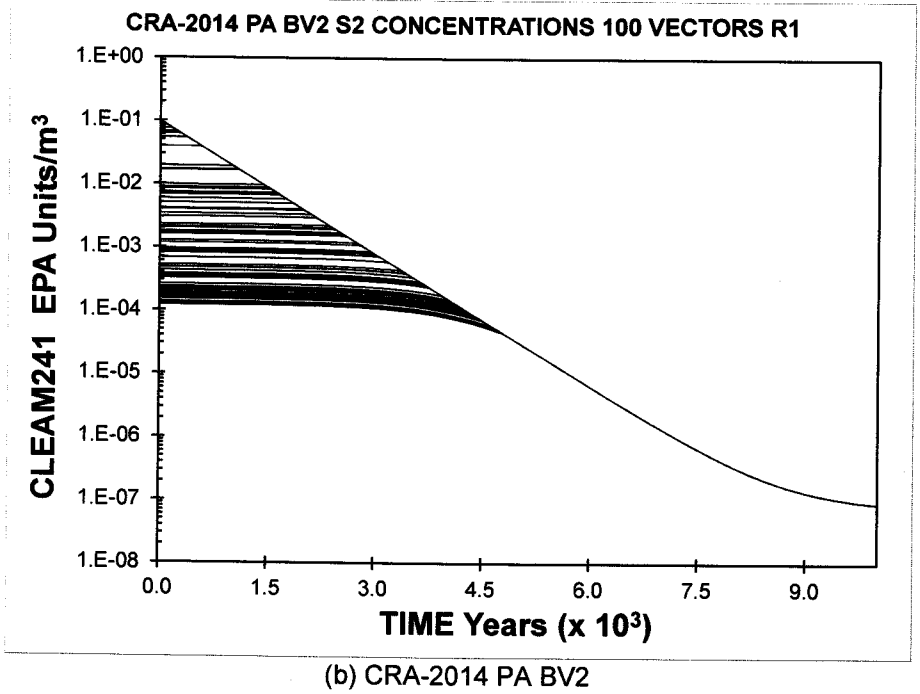


(f) CRA-2009 PABC

Figure 49 (*continued*). Time dependent total concentrations in Castile brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

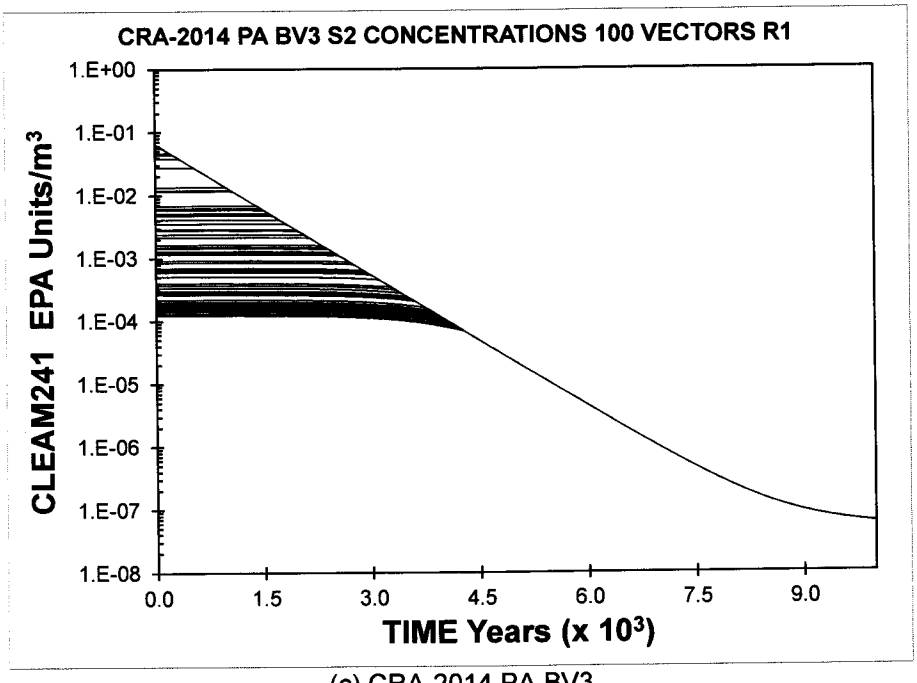


(a) CRA-2014 PA BV1

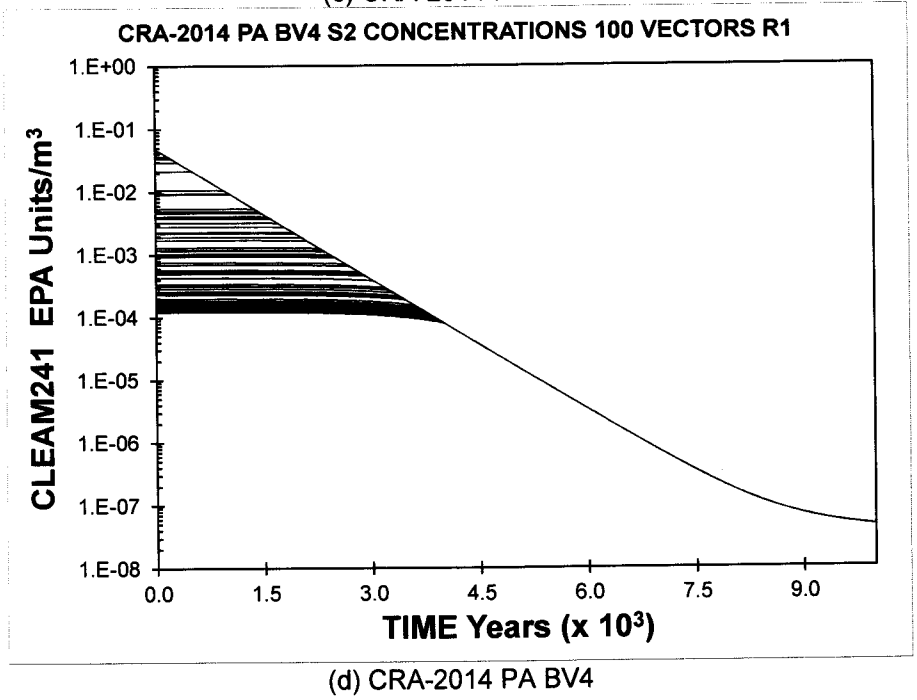


(b) CRA-2014 PA BV2

Figure 50. Time dependent AM241L concentration in Castile brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

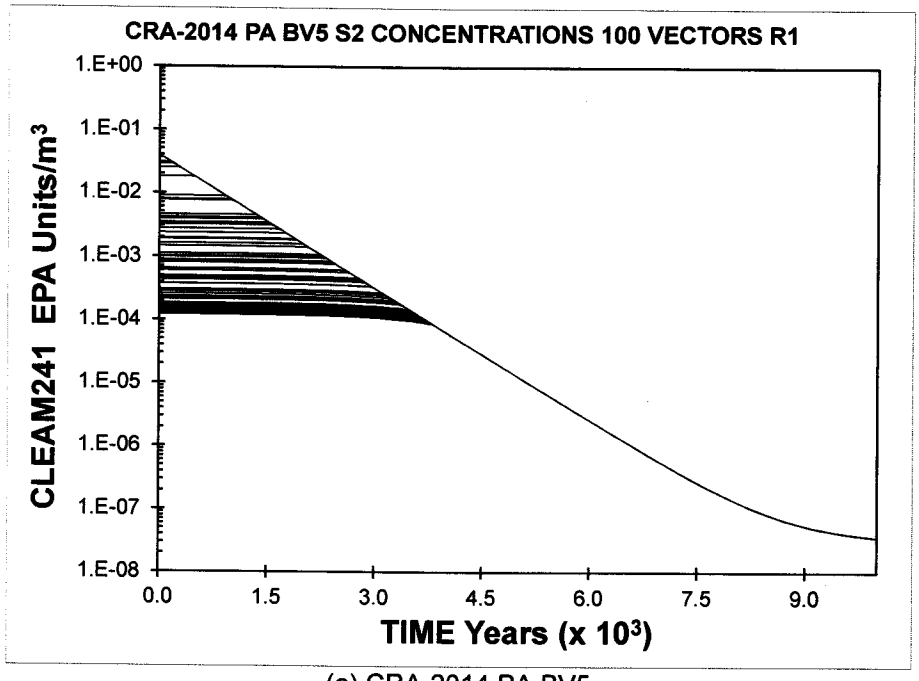


(c) CRA-2014 PA BV3

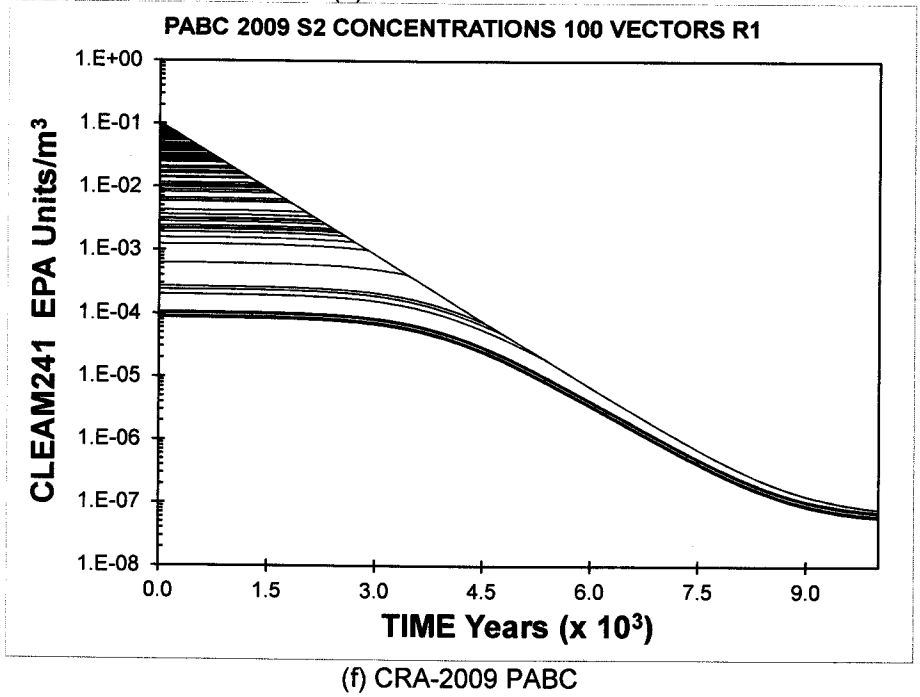


(d) CRA-2014 PA BV4

Figure 51 (*continued*). Time dependent AM241L concentration in Castile brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

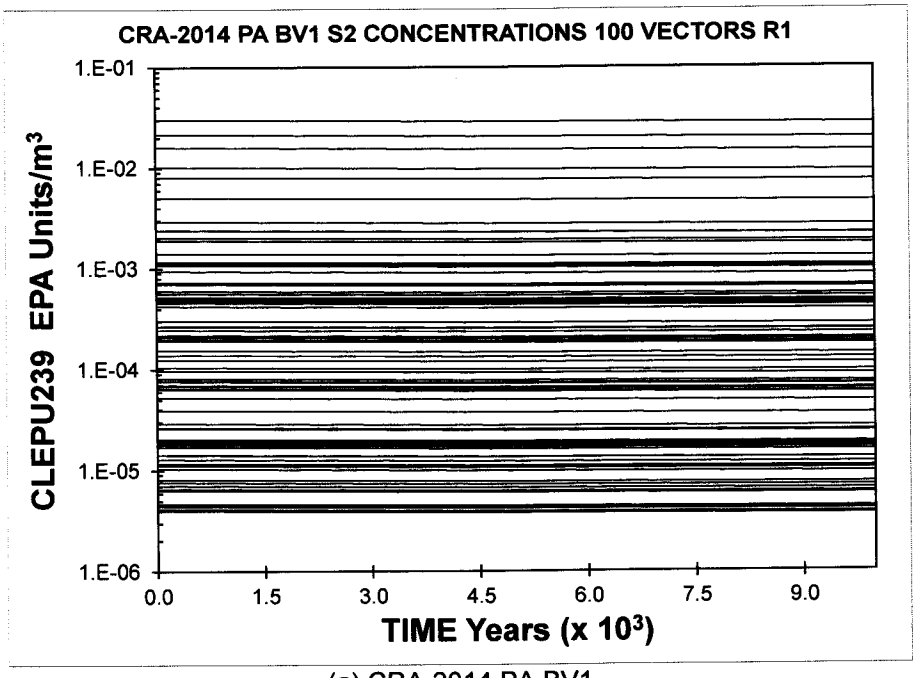


(e) CRA-2014 PA BV5

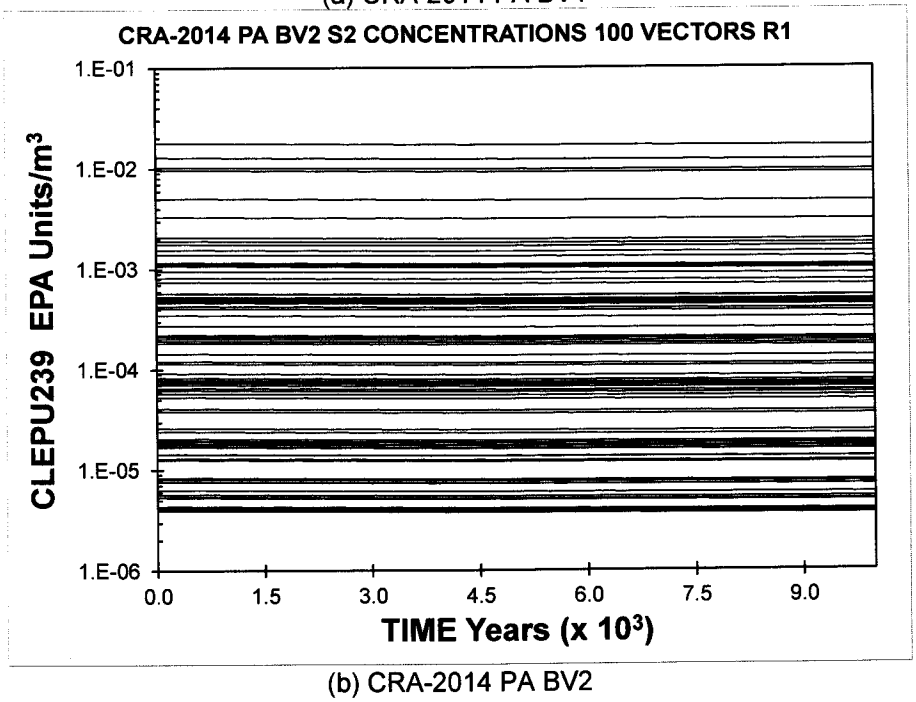


(f) CRA-2009 PABC

Figure 52 (*continued*). Time dependent AM241L concentration in Castile brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

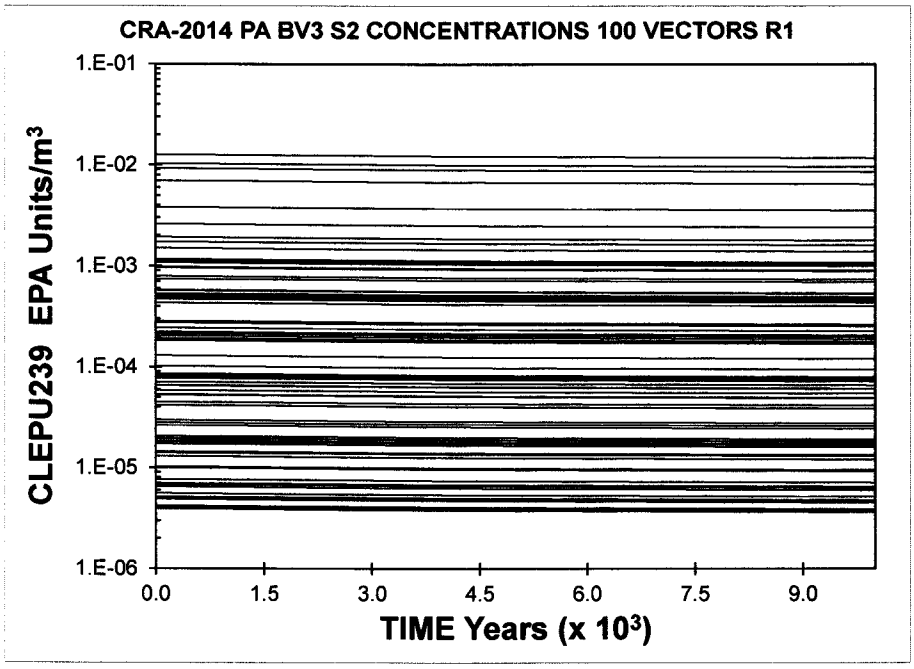


(a) CRA-2014 PA BV1

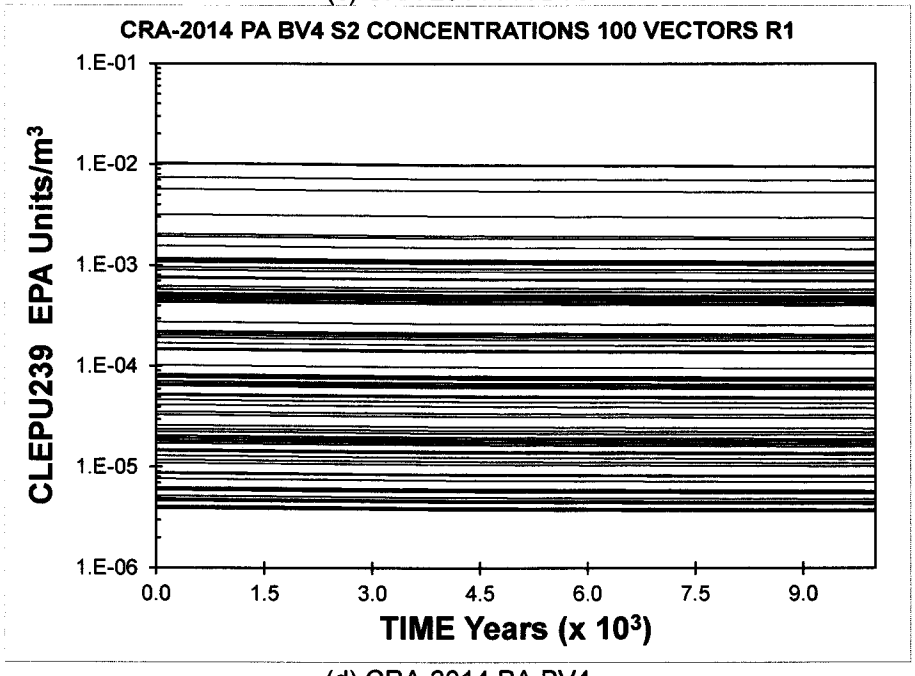


(b) CRA-2014 PA BV2

Figure 53. Time dependent PU239L concentration in Castile brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

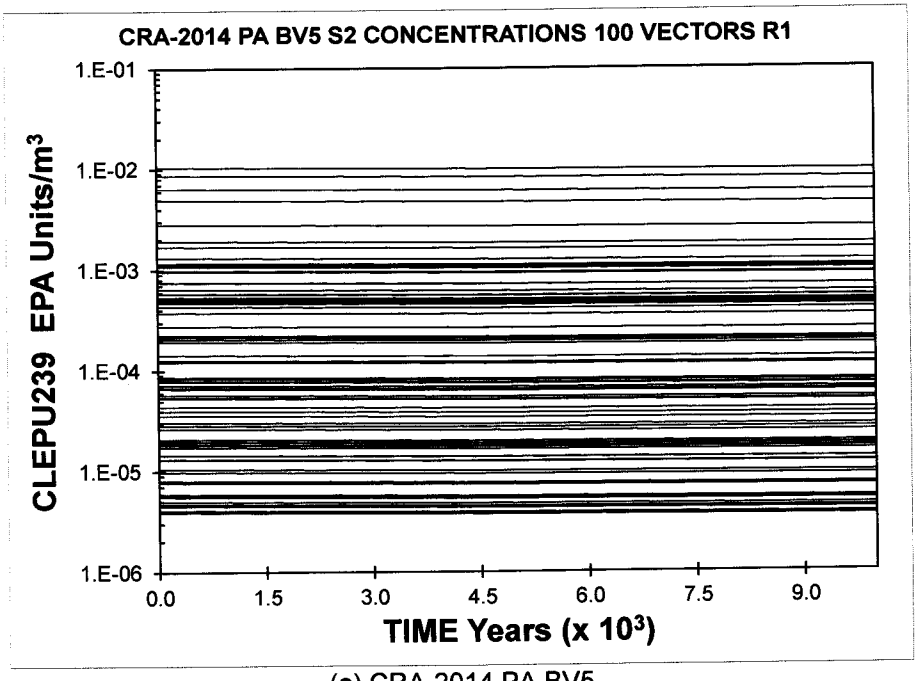


(c) CRA-2014 PA BV3

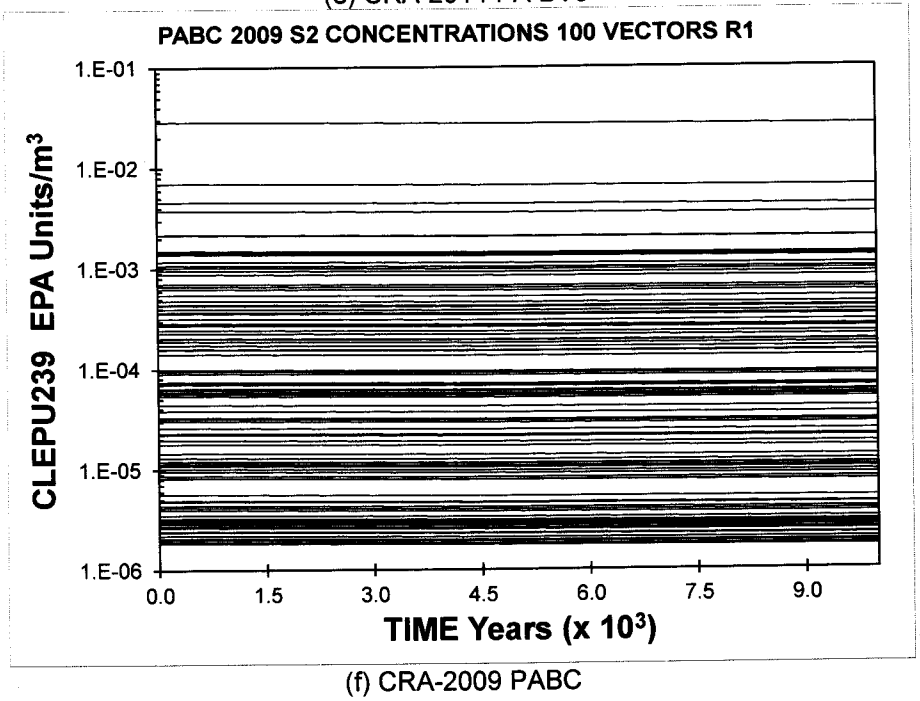


(d) CRA-2014 PA BV4

Figure 54 (*continued*). Time dependent PU239L concentration in Castile brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

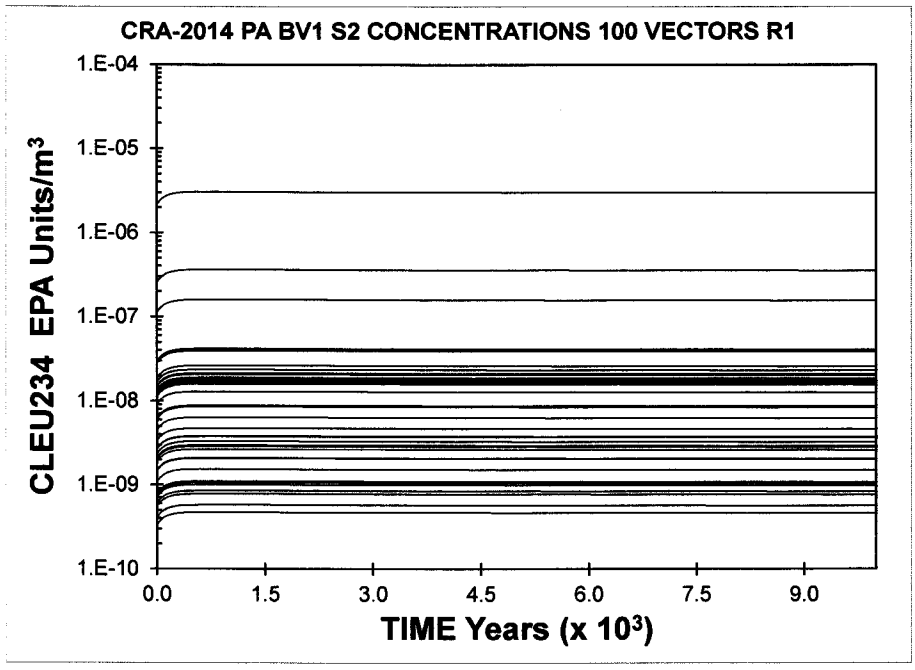


(e) CRA-2014 PA BV5

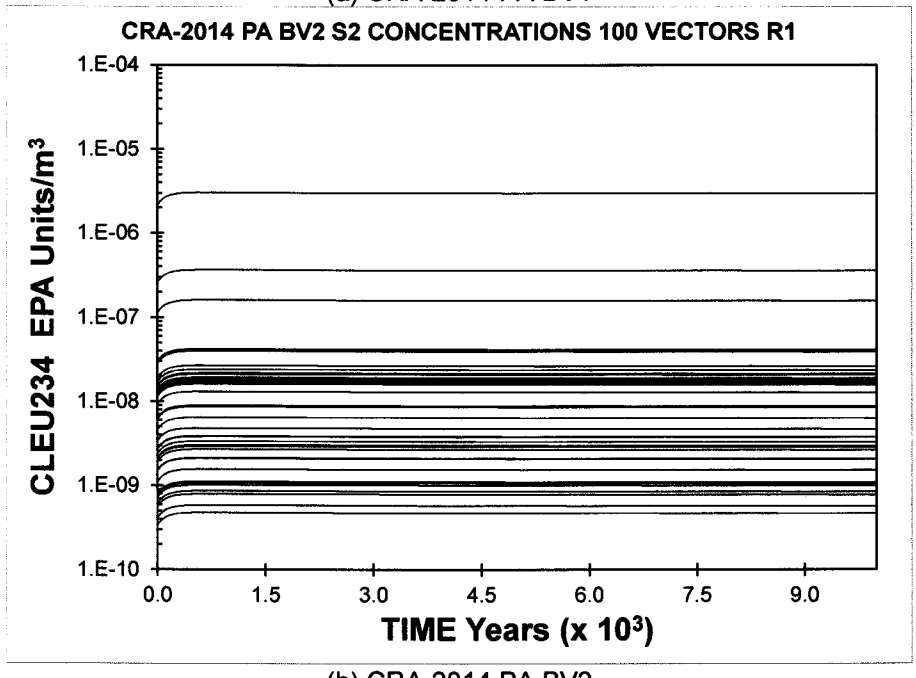


(f) CRA-2009 PABC

Figure 55 (*continued*). Time dependent PU239L concentration in Castile brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

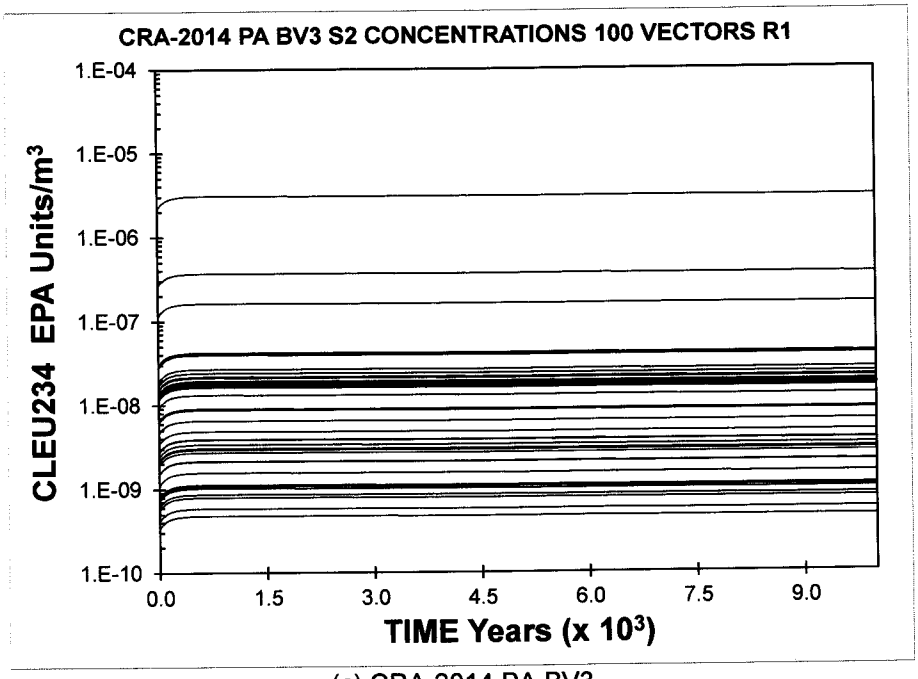


(a) CRA-2014 PA BV1

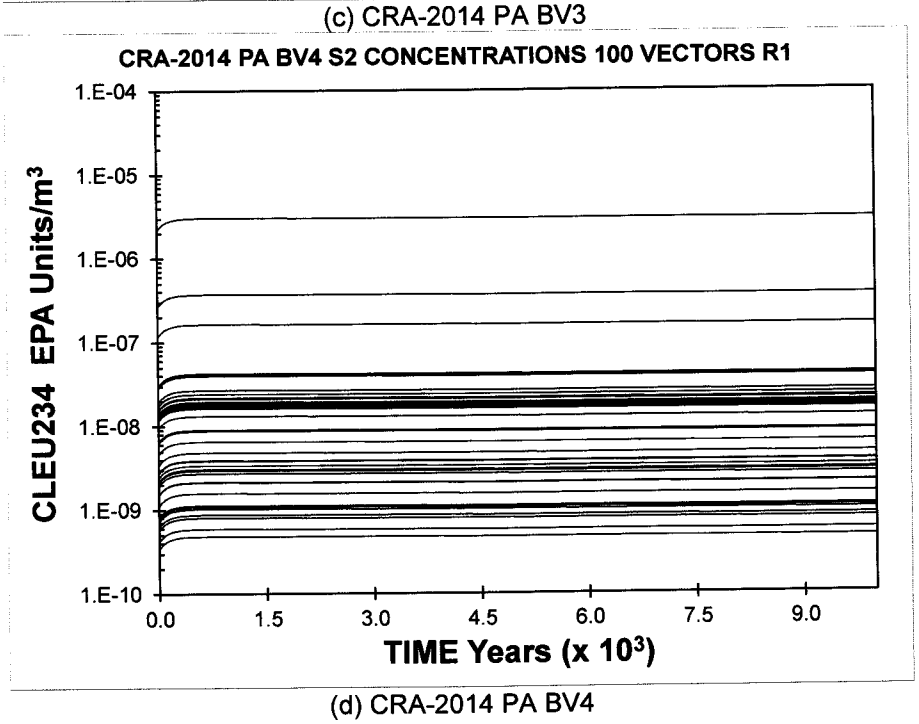


(b) CRA-2014 PA BV2

Figure 56. Time dependent U234L concentration in Castile brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

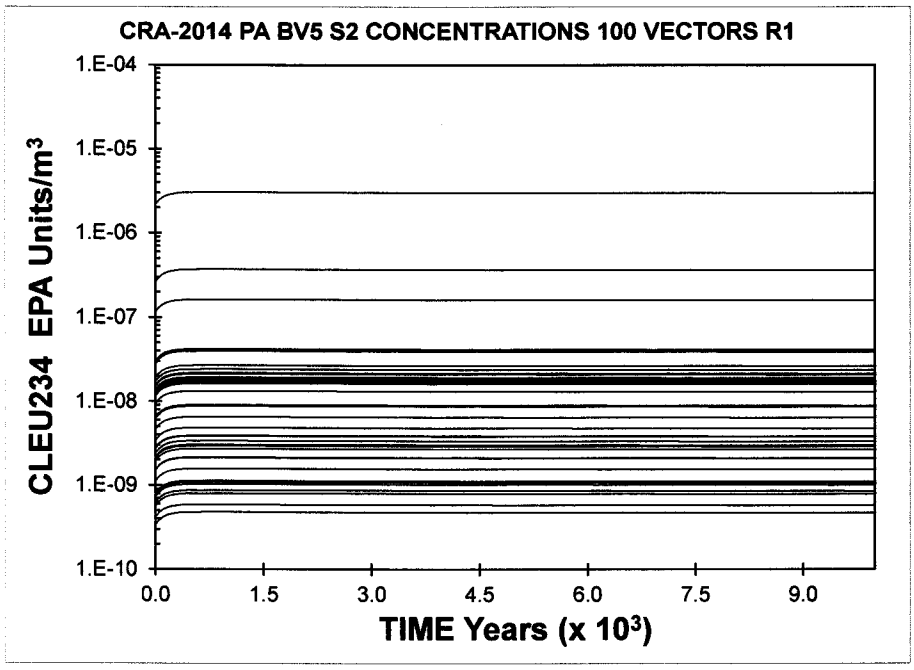


(c) CRA-2014 PA BV3

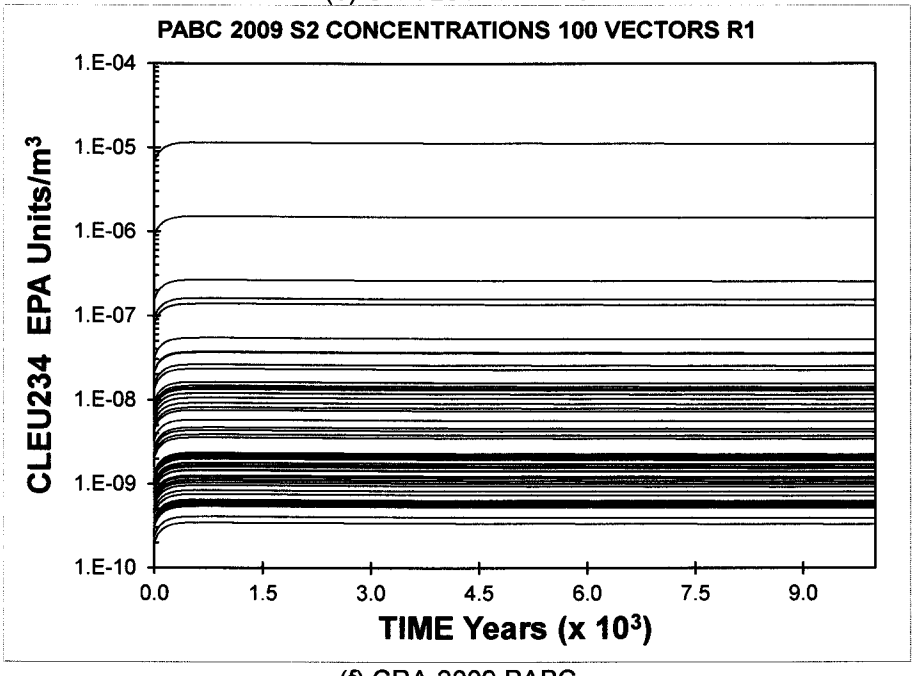


(d) CRA-2014 PA BV4

Figure 57 (*continued*). Time dependent U234L concentration in Castile brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

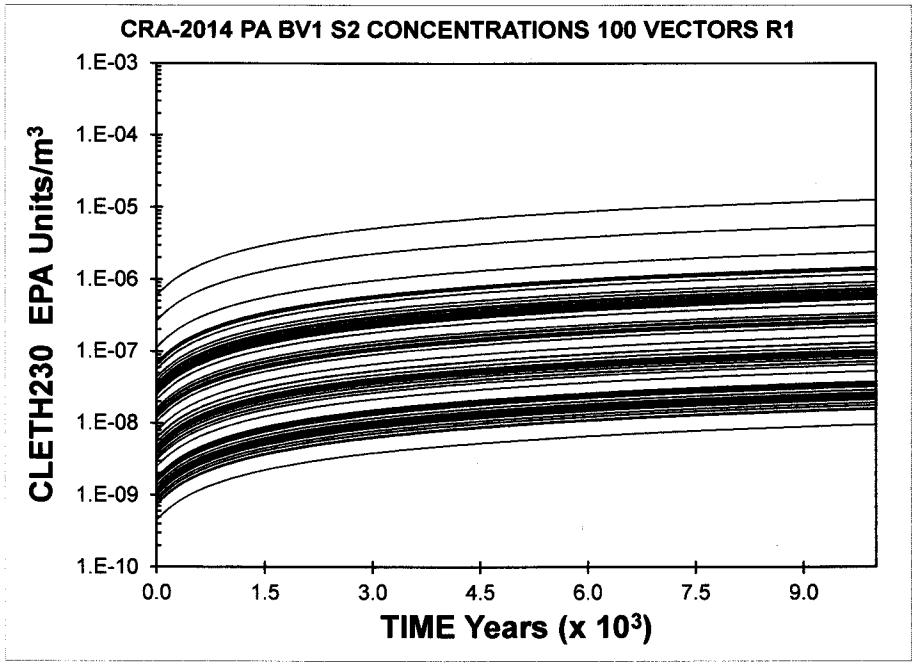


(e) CRA-2014 PA BV5

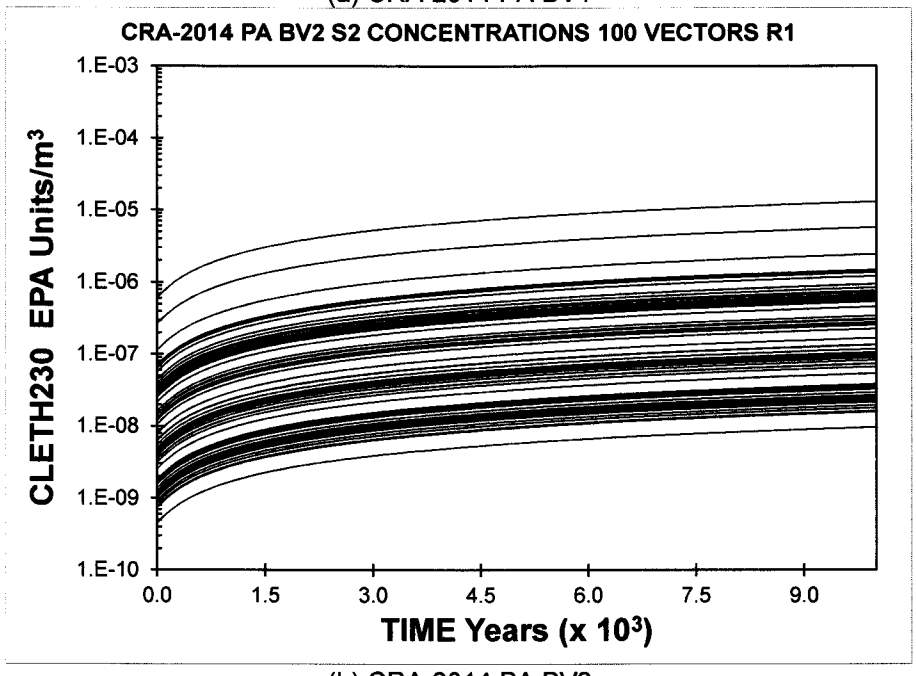


(f) CRA-2009 PABC

Figure 58 (*continued*). Time dependent U234L concentration in Castile brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

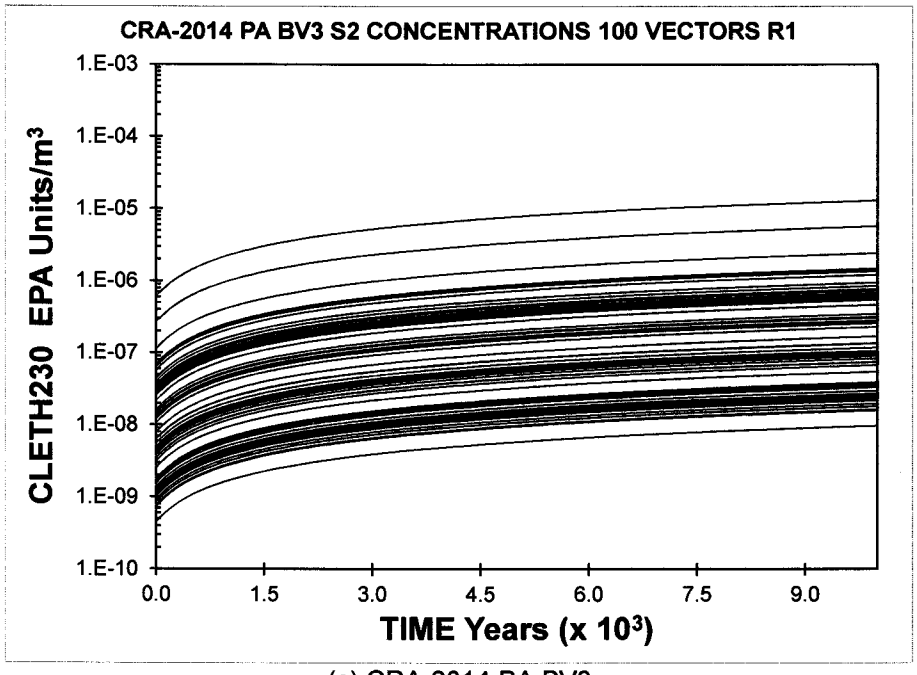


(a) CRA-2014 PA BV1

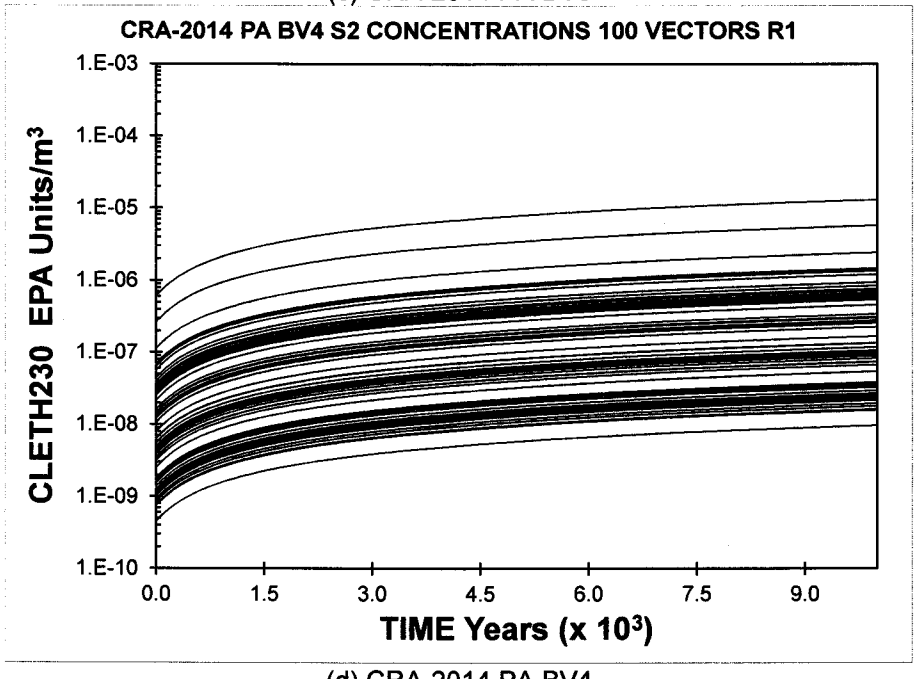


(b) CRA-2014 PA BV2

Figure 59. Time dependent TH230L concentration in Castile brine, where (a) BV1 and (b) BV2. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

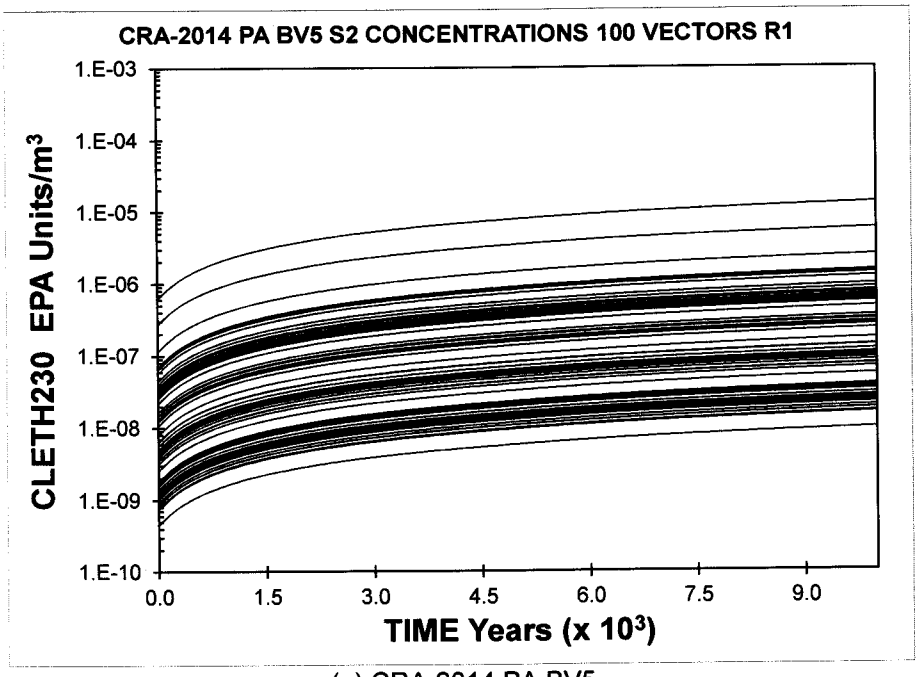


(c) CRA-2014 PA BV3

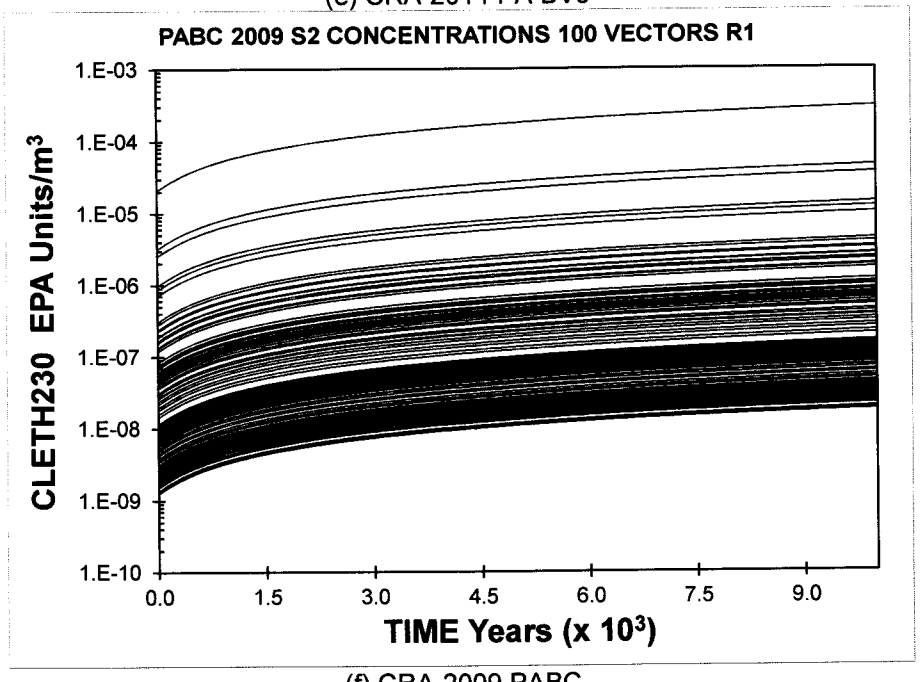


(d) CRA-2014 PA BV4

Figure 60 (*continued*). Time dependent TH230L concentration in Castile brine, where (c) BV3 and (d) BV4. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.



(e) CRA-2014 PA BV5



(f) CRA-2009 PABC

Figure 61 (*continued*). Time dependent TH230L concentration in Castile brine, where (e) BV5 and (f) CRA-2009 PABC. Part (a)-(e) shows results from the CRA-2014 PA. Part (f) shows results from the CRA-2009 PABC.

5.4 RADIONUCLIDES UP THE BOREHOLE (S6)

PANEL is run in the STANDARD mode for the S6 scenario to determine the EPA units up the borehole to the Culebra. PANEL calculates the mobilized radionuclide concentrations using panel brine volumes and brine flow volumes from BRAGFLO. The volume of brine in the panel and the flow of brine past the disturbed rock zone (DRZ) of the Salado are obtained from the POSTBRAG runs of BRAGFLO results. It is assumed that any brine that gets past the DRZ gets to the Culebra instantly.

The PANEL results for the EPA units up the borehole to the Culebra are not included in this document. They are listed in the NUTS/PANEL 2014 (Kim, 2013).

6. REFERENCES

Babb, S.C., and C.F. Novak. 1997 and addenda. *User's Manual for FMT Version 2.3: A Computer Code Employing the Pitzer Activity Coefficient Formalism for Calculating Thermodynamic Equilibrium in Geochemical Systems to High Electrolyte Concentrations.* Albuquerque, NM. Sandia National Laboratories. ERMS #243037.

Baker, B.L. 2003a. *Software Installation and Checkout Form for STEPWISE, Version 2.21.* Carlsbad, NM. Sandia National Laboratories. ERMS #526232.

Baker, B.L. 2003b. *Software Installation and Checkout Form for SPLAT, Version 1.02.* Carlsbad, NM. Sandia National Laboratories. ERMS #526231.

Baker, B.L. 2003c. *Software Instillation and Checkout Form for SUMMARIZE, Version 2.20.* ERMS #526233.

Bateman, H. 1910. The Solution of a System of Differential Equations Occurring in the Theory of Radio-active Transformations, Proc. Cambridge Phil. Soc. 16, 423. ERMS #249326.

Brush, L.H. 2005. "Results of Calculations of Actinide Solubilities for the WIPP Performance Assessment Baseline Calculations." Analysis report, May 18, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS #539800.

Brush, L.H. 2013. "Th(IV), Np(V), and Am(III) Baseline Solubilities and Th(IV) and Am(III) Solubility Uncertainties for the CRA-2014 PA." Memo to Chris Camphouse, Carlsbad, NM: Sandia National Laboratories. ERMS# 559279.

Brush, L.H., and P.S. Domski, 2013a. "Prediction of Baseline Actinide Solubilities for the WIPP CRA-2014 PA." Analysis Plan AP-153, January 21, 2013. Carlsbad, NM: Sandia National Laboratories. ERMS# 559138.

Brush, L.H., and P.S. Domski, 2013b. "Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2014 PA, Rev.1 Supersedes ERMS 559278." Analysis Plan AP-153, April 5, 2013. Carlsbad, NM: Sandia National Laboratories. ERMS# 559712.

Brush, L.H., P.S. Domski, and Y.-L. Xiong. 2012a. "Analysis Plan for WIPP Near-Field Geochemical Process Modeling." AP-153, Rev. 1, February 8, 2012. Carlsbad, NM: Sandia National Laboratories. ERMS# 556960.

Brush, L.H., P.S. Domski, and Y.-L. Xiong. 2012b. "Revised Predictions of WIPP Baseline Actinide Solubilities as a Function of the Volume of Standard Brines." Analysis report, May 17, 2012. Carlsbad, NM: Sandia National Laboratories. ERMS# 557524.

Brush, L.H., and Y.-L. Xiong, 2005a. "Calculation of Actinide Solubilities for the WIPP Performance-Assessment Baseline Calculations, Analysis Plan AP-120, Rev. 0." April 4, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS #539255.

Brush, L.H., and Y.-L. Xiong, 2005b. "Calculation of Organic-Ligand Concentrations for the WIPP Performance-Assessment Baseline Calculations." Analysis report, May 4, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS #539635.

Brush, L.H., and Y.-L. Xiong, 2009a. "Analysis Plan for the Calculation of Actinide Solubilities for the WIPP CRA-2009 PABC." Analysis Plan AP-143, May 6, 2009. Carlsbad, NM: Sandia National Laboratories. ERMS #551179.

Brush, L.H., and Y.-L. Xiong, 2009b. "Calculation of Organic-Ligand Concentrations for the WIPP CRA-2009 PABC." Analysis Report, June 16, 2009. Carlsbad, NM: Sandia National Laboratories. ERMS #551481.

Brush, L.H., and Y.-L. Xiong, 2009c. "Results of the Calculations of Actinide Solubilities for the CRA-2009 PABC." Analysis Report, October 7, 2009. Carlsbad, NM: Sandia National Laboratories. ERMS #552201.

Camphouse, R.C. 2013. Analysis Plan for the 2014 WIPP Compliance Recertification Application Performance Assessment. Sandia National Laboratories, Carlsbad, NM. ERMS 559198.

Clayton, D.J. 2008. "Update to the Calculation of the Minimum Brine Volume for a Direct Brine Release." Memorandum to L.H. Brush, April 2, 2008. Carlsbad, NM: Sandia National Laboratories. ERMS #548522.

Clayton, D.J., S. Dunagan, J.W. Garner, A.E. Ismail, T.B. Kirchner, G.R. Kirkes, M.B. Nemer. 2008. Summary Report of the 2009 Compliance Recertification Application Performance Assessment. Sandia National Laboratories, Carlsbad, NM. ERMS #548862.

Clayton, D.J. 2009a. Modifications to PANEL calculation sequence to include automatic calculation of the LSOLDIFF values. Carlsbad, NM. Sandia National Laboratories, ERMS #551947.

Clayton, D.J. 2009b. Analysis Plan for the CRA-2009 Performance Assessment Baseline Calculation. Carlsbad, NM. Sandia National Laboratories, ERMS #551603.

Clayton, D.J., R.C. Camphouse, J.W. Garner, A.E. Ismail, T.B. Kirchner, K.L. Kuhlman, M.B. Nemer. 2010. Summary Report of the CRA-2009 Performance Assessment Baseline Calculation. Sandia National Laboratories, Carlsbad, NM. ERMS 553039.

Cotsworth, E. 2005. *EPA letter on conducting the performance assessment baseline change (PABC) verification test.* Washington, D.C. U.S. EPA, Office of Radiation and Indoor Air. ERMS #538858.

Cotsworth, E. 2009. EPA Letter on CRA-2009 First Set of Completeness Comments. U.S. EPA, Office of Radiation and Indoor Air, Washington, D.C. ERMS #551444.

Crawford, B.A., D. Guerin, S. Lott, B. McInroy, J. McTaggart, and G. Van Soest. 2009. "Performance Assessment Inventory Report – 2008." INV-PA-08, Rev 0. Carlsbad, NM: LA-UR-09-02260, Los Alamos National laboratory – Carlsbad Operations. ERMS #551509.

Fox, B., D. Clayton, T. Kirchner. Radionuclide Inventory Screening Analysis Report for the PABC – 2009, 7/20/2009, ERMS #551679

Garner, J.W. 1998. "WIPP PA Validation Document for PANEL Version 4.00", January 13, 1998, Carlsbad, NM: Sandia National Laboratories. WPO# 48791.

Garner, J.W. 2003a. "Change Control Form for PANEL Version 4.00." Carlsbad, NM: Sandia National Laboratories. ERMS# 526499.

Garner, J.W. 2003b. "Users Manual for PANEL Version 4.02." Carlsbad, NM: Sandia National Laboratories. ERMS# 526652.

Garner, J.W. 2003c. "Validation Document for PANEL Version 4.02." Carlsbad, NM: Sandia National Laboratories. ERMS# 526650.

Garner, J.W. 2005a. "Change Control Form for PANEL Version 4.02." Carlsbad, NM: Sandia National Laboratories. ERMS # 539537.

Garner, J.W. 2005b. *Parameter Data Entry for SOLMOD4, SOLVAR CRA1BC.* Carlsbad, NM. Sandia National Laboratories. ERMS# 539652.

Garner, J.W. 2005c. *Parameter Data Entry For SOLMOD3, SOLVAR CRA1BC.* Carlsbad, NM: Sandia National Laboratories. ERMS# 539651.

Graner, J.W. 2010. "Analysis Package for PANEL: CRA-2009 Performance Assessment Baseline Calculation." Carlsbad, NM: Sandia National Laboratories. ERMS# 553032.

Gilkey, A.P. 2003a. *Software Installation and Checkout Form for ALGEBRACDB, Version 2.35.* Carlsbad, NM. Sandia National Laboratories. ERMS #526236.

Gilkey, A.P. 2003b. *Software Installation and Checkout Form for MATSET, Version 9.10.* Carlsbad, NM. Sandia National Laboratories. ERMS# 526219.

Helton, J.C., J.E. Bean, J.W. Berglund, F.J. Davis, K. Economy, J.W. Garner, J.D. Johnson, R.J. MacKinnon, J. Miller, D.G. O'Brien, J.L. Ramsey, J.D. Schreiber, A. Shinta, L.N. Smith, D.M. Stoelzel, C. Stockman, and P. Vaughn. 1998. "Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant." SAND98-0365. Albuquerque, NM: Sandia National Laboratories. ERMS #252619.

Kaplan, Irving 1964. Nuclear Physics, 2nd Ed. (Chapter 10), Addison-Wesley Publishing Co, Reading, Mass. ERMS #242558.

Kicker, D.C., T. Zeitler. 2013. "Radionuclide Inventory Screening Analysis for the 2014 Compliance Recertification Application Performance Assessment (CRA-2014 PA)", February 19, 2013, Carlsbad, NM: Sandia National Laboratories, ERMS# 559257.

Kim, S. 2013. "Analysis Package for Salado Transport Calculations: CRA-2014 Performance Assessment", May, 2013, Carlsbad, NM: Sandia National Laboratories, ERMS #.

Lappin. A.R., R.L. Hunter, D.P. Garber, P.B. Davies. 1989. *Systems Analysis, Long-Term Radionuclide Transport, and Dose Assessments, Waste Isolation Pilot Plant (WIPP), Southeastern New Mexico; March 1989.* SAND89-0462. Albuquerque, NM. Sandia National Laboratories. ERMS #224125.

Leigh, C.D. 2003. *Software Installation and Checkout Form for NUTS, Version 2.05A.* Carlsbad, NM. Sandia National Laboratories. ERMS #526220.

Leigh, C.D., J.F. Kanney, L.H. Brush, J.W. Garner, G.R. Kirkes, T. Lowry, M.B. Nemer, J.S. Stein, E.D. Vugrin, S. Wagner, and T.B. Kirchner. 2005. 2004 Compliance Recertification Application Performance Assessment Baseline Calculation, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS #541521.

Leigh, C.D. and J.R. Trone. 2005a. *Calculation of Radionuclide Inventories for Use in NUTS in the Performance Assessment Baseline Calculation.* Carlsbad, NM. Sandia National Laboratories. ERMS #539644.

Leigh, C.D. and J.R. Trone. 2005b. *Calculation of the Waste Unit Factor For the Performance Assessment Baseline Calculation, Revision 0.* Carlsbad, NM. Sandia National Laboratories. ERMS #539644.

Long, J.J. 2013. "Run Control - Execution of Performance Assessment Codes for the CRA-2014 Performance Assessment", 2013, Carlsbad, NM: Sandia National Laboratories. ERMS# 560016.

MacKinnon, R.J., and G. Freeze. 1997a. Summary of EPA-Mandated Performance Assessment Verification Test (Replicate 1) and Comparison With the Compliance Certification Application Calculations, Revision 1. Sandia National Laboratories, Carlsbad, NM. ERMS #422595

MacKinnon, R.J., and G. Freeze. 1997b. Summary of Uncertainty and Sensitivity Analysis Results for the EPA-Mandated Performance Assessment Verification Test, Rev. 1. Sandia National Laboratories, Carlsbad, NM. ERMS #420669.

MacKinnon, R.J., and G. Freeze. 1997c. Supplemental Summary of EPA-Mandated Performance Assessment Verification Test (All Replicates) and Comparison With the Compliance Certification Application Calculations, Revision 1. Sandia National Laboratories, Carlsbad, NM. ERMS #414880.

Nemer, M.B. 2006. *Users Manual for BRAGFLO, Version 6.00.* Carlsbad, NM. Sandia National Laboratories. ERMS # 545016.

Papenguth, H. W. 1996a. PRP: Mobile Colloidal Actinide Source Term. 2. Actinide Intrinsic Colloids. Carlsbad, NM: Sandia National Laboratories. ERMS# 235852.

Papenguth, H. W. 1996b. Memo: H. Papenguth to C. Stockman, 3/29/96, Colloidal Actinide Source Term Parameters. Carlsbad, NM: Sandia National Laboratories. ERMS# 236771.

Roselle, G. 2013. *Summary of colloid parameters to be implemented in the CRA-2014 PA.* Carlsbad, NM: Sandia National Laboratories. ERMS# 559205.

Stein, J.S. 2005. *Estimate of Volume of Brine in Repository That Leads to a Brine Release.* Carlsbad, NM. Sandia National Laboratories. ERMS #539372.

Stein, J.S. 2003a. *Software Installation and Checkout Form for BRAGFLO, Version 5.0.* Carlsbad, NM. Sandia National Laboratories. ERMS #525704.

Stein, J.S. 2003b. *Software Installation and Checkout Form for POSTBRAG, Version 4.00.* Carlsbad, NM. Sandia National Laboratories. ERMS #526223.

Stein, J.S. 2003c. *Software Installation and Checkout Form for GENMESH, Version 6.08.* ERMS # 526215. Carlsbad, NM. Sandia National Laboratories.

Tierney, M. 1996. *Form 464, ID 3429, IDMTRL PHUMOX3, IDPRAM PHUMCIM.* Carlsbad, NM. Sandia National Laboratories. ERMS #237683.

Tisinger, S. 2002. Software Installation and Checkout Form for PAPDB, Version 1.00. Carlsbad, NM. Sandia National Laboratories. ERMS #518619.

U.S. Congress. 1992. WIPP Land Withdrawal Act, Public Law 102-579, 106 Stat. 4777, 1992; as amended by Public Law 104-201, 110 Stat. 2422, 1996.

U. S. DOE 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant.* DOE/CAO-1996-2184. U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office, Carlsbad, NM.

U.S. DOE 2004. *Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot.* DOE/WIPP 2004-3231, 10 vols., U.S. Department of Energy Waste Isolation Pilot Plant, Carlsbad Field Office, Carlsbad, NM.

U.S. DOE 2009. *Title 40 CFR Part 191 Subparts B and C Compliance Recertification Application for the Waste Isolation Pilot Appendix MgO-2009 Magnesium Oxide as an Engineered Barrier.* DOE/WIPP-09-3424, U.S. Department of Energy Waste Isolation Pilot Plant, Carlsbad Field Office, Carlsbad, NM.

U.S. Environmental Protection Agency (EPA). 1998. 40 CFR 194, Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the Disposal Regulations: Certification Decision: Final Rule. Federal Register, Vol. 63, 27354-27406. ERMS #251924.

U.S. Environmental Protection Agency (EPA). 2006. 40 CFR 194, Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the Disposal Regulations: Certification Decision: Final Rule, Federal Register. Vol. 71, 18010-18021.

U.S. Environmental Protection Agency (EPA). 2010. 40 CFR Part 194 Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance With the Disposal Regulations: Recertification Decision, Federal Register No. 222, Vol. 75, pp. 70584-70595, November 18, 2010.

Van Soest, G.D. 2012. *Performance Assessment Inventory Report – 2012.* INV-PA-12, Revision 0. Los Alamos National Laboratory, Carlsbad, NM. LA-UR-12-26643.

Vugrin, E.D. 2005a. "Software Installation and Checkout and Analysis Report for the ES45 Regression Test of LHS, Version 2.42." Carlsbad, NM: Sandia National Laboratories. ERMS# 538376.

Vugrin, E.D. 2005b. *Software Installation and Checkout and Installation and Checkout for POSTLHS, Version 4.07A Regression Testing for the COMPAQ ES40 and ES45 Platforms.* Carlsbad, NM. Sandia National Laboratories. ERMS #539483.

Vugrin, E.D. 2004. *Software Installation and Checkout and Analysis Report for the ES45 Regression Test of CCDFGF, Version 5.02.* Carlsbad, NM. Sandia National Laboratories. ERMS #538169.

Wang, Y. 1998. *WIPP PA Validation Document for FMT (Version 2.4), Document Version 2.4.* Carlsbad, NM. Sandia National Laboratories. ERMS #251587.

Wolery, T.J. 2008. "Analysis Plan for EQ3/6 Analytical Studies." AP-140, Rev. 0, May 15, 2008, Carlsbad, NM: Sandia National Laboratories. ERMS# 548930.

Wolery, T.J., and R.L. Jarek. 2003. "Software User's Manual: EQ3/6, Version 8.0." Software Document No. 10813-UM-8.0-00. Albuquerque, NM: Sandia National Laboratories.

Wolery, T.J., Y.-L. Xiong, and J.J.Long. 2010. "Verification and Validation Plan/Validation Document for EQ3/6 Version 8.0a for Actinide Chemistry, Document Version 8.10." Carlsbad, NM: Sandia National Laboratories. ERMS# 550239.

Xiong, Y.-L. 2011a. "Release of EQ3/6 Database DATA0.FM1." E-mail to Jennifer Long, March 9, 2011. Carlsbad, NM: Sandia National Laboratories. ERMS# 555152.

Xiong, Y.-L. 2011b. "WIPP Verification and Validation Plan/Validation Document for EQ3/6 Version 8.0a for Actinide Chemistry, Revision 1. Supersedes ERMS 550239." May 12, 2011. Carlsbad, NM: Sandia National Laboratories. ERMS# 555358.

Xiong, Y.L., L.H. Brush, A.E. Ismail, and J.J. Long. 2009. *Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2009 PABC.* Analysis report, December 1, 2009. Carlsbad, NM: Sandia National Laboratories. ERMS #552500.

Xiong, Y.-L., E.J. Nowak, and L.H. Brush. 2005. *Updated Uncertainty Analysis of Actinide Solubilities for the Response to EPA Comment C-23-16* (Supersedes ERMS #538219). Analysis report, April 29, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS #539595.

APPENDIX A: CALCULATION OF LSOLDIF

PANEL supplies information from the CONCENTRATION run to NUTS. For NUTS the values supplied by PANEL are defined in Equation 11 (see Section 3.3).

$$\left\{TC_{brine}^{red/ox}\right\}_{NUTS} = TC_{brine}^{red/ox} \bullet 10^{-L_{dif}^{sol}} \tag{11}$$

where $\left\{TC_{brine}^{red/ox}\right\}_{NUTS}$ is the potential moles per liter mobilized for the lumped isotopes in Table 11 (see Section 3.3). L_{dif}^{sol} is a multiplicative factor used to account for molar proportions of isotopes in the inventory. $TC_{brine}^{red/ox}$ is an elemental value. It is the potential moles per liter mobilized of an element. It is assumed that isotopes of an element are mobilized in proportion to their molar proportions in the inventory. For example U in the WIPP PA inventory is comprised of several isotopes including but not limited to U235, U238, U232, and U236. Of these, U238 has the highest molar proportions in the inventory. Therefore, for every mole of U that is mobilized, there is more U238 mobilized than any other U isotope.

U234L is defined as the amount of U234 plus the amount of U233. Therefore, L_{dif}^{sol} for U234L is defined as:

$$\left(L_{dif}^{sol}\right)_{U234L} = -\log\left\{\frac{N^{U233} + N^{U234}}{\sum_i N^{isotope}}\right\} \tag{A.1}$$

N^{U233} and N^{U234} are the total moles U233 and U234 in the inventory, respectively. $\sum_i N^{isotope}$ is the sum of all isotopes of the element that contains the isotopes of interest. PU238L is defined as the amount of PU238. Therefore, L_{dif}^{sol} for PU238L is defined as:

$$\left(L_{dif}^{sol}\right)_{PU238L} = -\log\left\{\frac{N^{PU238}}{\sum_i N^{isotope}}\right\} \tag{A.2}$$

N^{PU238} is the moles of PU238 in the inventory. TH230L is defined as the amount of TH230 plus the amount of TH229. Therefore, L_{dif}^{sol} for TH230L is defined as

$$\left(L_{dif}^{sol}\right)_{TH230L} = -\log\left\{\frac{N^{TH229} + N^{TH230}}{\sum_i N^{isotope}}\right\} \tag{A.3}$$

N^{TH229} and N^{TH230} are the total moles TH229 and TH230 in the inventory, respectively. AM241L is defined as the amount of AM241 plus the amount of PU241. Since AM241 is the predominant isotope for Am and PU241 quickly decays to Am241, the potential moles per liter mobilized for AM241L is defined as:

$$\left\{TC_{brine}^{red/ox}\right\}_{AM241L} = \left\{TC_{brine}^{red/ox}\right\}_{Am} \quad \text{(A.4)}$$

There is no L_{dif}^{sol} for AM241L. PU239L is defined as the amount of PU239 plus the amount of PU240 plus the amount of PU242 which accounts for almost all of the Pu in the inventory. Therefore, the potential moles per liter mobilized for PU239L is defined as:

$$\left\{TC_{brine}^{red/ox}\right\}_{PU239L} = \left\{TC_{brine}^{red/ox}\right\}_{Pu} \quad \text{(A.5)}$$

There is no L_{dif}^{sol} for PU239L.

Because of radioactive decay and production, the value of L_{dif}^{sol} will change over time. For WIPP PA, a single value for L_{dif}^{sol} is chosen, the maximum value over time. The maximum value is found by running PANEL in the DECAY mode. Using the results from the PANEL DECAY run, L_{dif}^{sol} is calculated at every time step and the maximum value over time is chosen (Clayton, 2009a).

A.1 DECAY RUN CALCULATIONS FOR CRA-2014 PA

PANEL was run in the DECAY mode to produce decayed radionuclide. First, the analyst ran GENMESH which generates a single-element grid. The analyst ran MATSET which assigns the material property values needed by PANEL. The GENMESH binary file that was input into the MATSET code (**GM_PANEL_CRA14.CDB** located in CMS library **CRA14_PANEL** class ANALYSIS) and the MATSET input file (**MS_PANEL_CRA14.INP** located in CMS library **CRA14_PANEL** class ANALYSIS), provided the initial material map for the DECAY run. The output files **MS_PANEL_CRA14.CDB** is located in CMS library **CRA14_PANEL** class ANALYSIS).

PANEL was then run with the **MS_PANEL_CRA14.CDB** file. This produced **PANEL_DECAY_CRA14_R1_S1_V001.CDB** located in CMS library **CRA14_PANEL** class ANALYSIS.

ALGEBRACDB was then run with the **PANEL_DECAY_CRA14_R1_S1_V001.CDB** and **ALG1_PANEL_CRA14.INP** (located in CMS library **CRA14_PANEL** class ANALYSIS). The following is the ALGEBRACDB input file that was used (**ALG1_PANEL_CRA14.INP**).

```
!
! This input file is for the CRA14 calculation, AP-164
```

```
! This file calculates the total moles of U,Pu, and Th and the mole fractions
! of U233+U234, PU238, and TH229+TH230, as well as the maximum mole fractions
!
ALLTIMES
U_MOLE  = SDMU233/ATWEIGHT[27]+SDMU234/ATWEIGHT[28]+SDMU235/ATWEIGHT[29]+ &
          SDMU236/ATWEIGHT[30]+SDMU238/ATWEIGHT[31]
PU_MOLE = SDMPU238/ATWEIGHT[15]+SDMPU239/ATWEIGHT[16]+SDMPU240/ATWEIGHT[17]+ &
          SDMPU241/ATWEIGHT[18]+SDMPU242/ATWEIGHT[19]+SDMPU244/ATWEIGHT[20]
TH_MOLE = SDMTH229/ATWEIGHT[24]+SDMTH230/ATWEIGHT[25]+SDMTH232/ATWEIGHT[26]

MF_U  = (SDMU233/ATWEIGHT[27]+SDMU234/ATWEIGHT[28])/U_MOLE
MF_PU = SDMPU238/ATWEIGHT[15]/PU_MOLE
MF_TH = (SDMTH229/ATWEIGHT[24]+SDMTH230/ATWEIGHT[25])/TH_MOLE

LSD_U  = -LOG10(ENVMAX(MF_U))
LSD_PU = -LOG10(ENVMAX(MF_PU))
LSD_TH = -LOG10(ENVMAX(MF_TH))

EXIT
```

This produced the output **ALG1_PANEL_CRA14.CDB** located in CMS library **CRA14_PANEL** class ANALYSIS.

ALG1_PANEL_CRA14.CDB was then run through GROPECDB to produce the text file **ALG1_PANEL_CRA14.LIS** (located in directory PAWORK:[SHARED.SUNKIM.CRA14.AP_PANEL.PANEL_DECAY]).

A.2 RESULTS

Table A.1 shows the results of running **ALG1_PANEL_CRA14.INP** on **PANEL_DECAY_CRA14_R1_S1_V001.CDB**. Visual analysis of the 201 time steps shows that the largest mole fraction for U234L (Column 5 in Table A.1) occurs at 850 years. The value is 3.88478E-04. Therefore,

$$\left(L_{dif}^{sol}\right)_{U234L} = -\log(3.88478\text{E-}04) = 3.41063$$

The largest mole fraction for PU238L occurs at time 0 and is 2.90292E-03. Therefore,

$$\left(L_{dif}^{sol}\right)_{PU238L} = -\log(2.90292\text{E-}03) = 2.53716$$

The largest mole fraction for TH230L occurs at 10,000 years and is 1.85683E-04. Therefore,

$$\left(L_{dif}^{sol}\right)_{TH230L} = -\log(1.85683\text{E-}04) = 3.73123$$

Table 15. Mole Fraction of Lumped Isotopes Over Time

Time (Years)	Total Moles U	Total Moles Pu	Total Moles Th	Mole Fraction U234L	Mole Fraction PU238L	Mole Fraction TH230L
0	9.60805E+05	5.07984E+04	5.87435E+04	2.36441E-04	2.90292E-03	1.56702E-05
50	9.60926E+05	5.06531E+04	5.87435E+04	2.86453E-04	1.96130E-03	1.63509E-05
100	9.61032E+05	5.05454E+04	5.87436E+04	3.20115E-04	1.32414E-03	1.71260E-05
150	9.61127E+05	5.04504E+04	5.87436E+04	3.42765E-04	8.93753E-04	1.79644E-05
200	9.61214E+05	5.03628E+04	5.87437E+04	3.57998E-04	6.03166E-04	1.88448E-05
250	9.61297E+05	5.02802E+04	5.87437E+04	3.68236E-04	4.07020E-04	1.97531E-05
300	9.61376E+05	5.02011E+04	5.87438E+04	3.75108E-04	2.74641E-04	2.06797E-05
350	9.61453E+05	5.01242E+04	5.87438E+04	3.79714E-04	1.85309E-04	2.16182E-05
400	9.61528E+05	5.00491E+04	5.87439E+04	3.82793E-04	1.25030E-04	2.25641E-05
450	9.61602E+05	4.99750E+04	5.87440E+04	3.84844E-04	8.43570E-05	2.35146E-05
500	9.61675E+05	4.99018E+04	5.87440E+04	3.86202E-04	5.69146E-05	2.44677E-05
550	9.61748E+05	4.98292E+04	5.87441E+04	3.87094E-04	3.83991E-05	2.54221E-05
600	9.61820E+05	4.97571E+04	5.87441E+04	3.87672E-04	2.59069E-05	2.63769E-05
650	9.61892E+05	4.96854E+04	5.87442E+04	3.88039E-04	1.74786E-05	2.73315E-05
700	9.61963E+05	4.96139E+04	5.87442E+04	3.88263E-04	1.17923E-05	2.82855E-05
750	9.62034E+05	4.95427E+04	5.87443E+04	3.88392E-04	7.95587E-06	2.92387E-05
800	9.62105E+05	4.94717E+04	5.87443E+04	3.88457E-04	5.36754E-06	3.01907E-05
850	9.62176E+05	4.94010E+04	5.87444E+04	3.88478E-04	3.62129E-06	3.11417E-05
900	9.62247E+05	4.93304E+04	5.87445E+04	3.88470E-04	2.44314E-06	3.20913E-05
950	9.62317E+05	4.92600E+04	5.87445E+04	3.88443E-04	1.64829E-06	3.30397E-05
1000	9.62387E+05	4.91897E+04	5.87446E+04	3.88403E-04	1.11204E-06	3.39868E-05
1050	9.62457E+05	4.91197E+04	5.87446E+04	3.88354E-04	7.50247E-07	3.49325E-05
1100	9.62527E+05	4.90498E+04	5.87447E+04	3.88299E-04	5.06161E-07	3.58769E-05
1150	9.62597E+05	4.89800E+04	5.87447E+04	3.88241E-04	3.41485E-07	3.68199E-05
1200	9.62666E+05	4.89104E+04	5.87448E+04	3.88180E-04	2.30385E-07	3.77615E-05
1250	9.62736E+05	4.88410E+04	5.87448E+04	3.88117E-04	1.55431E-07	3.87018E-05
1300	9.62805E+05	4.87718E+04	5.87449E+04	3.88054E-04	1.04862E-07	3.96407E-05
1350	9.62874E+05	4.87027E+04	5.87450E+04	3.87990E-04	7.07457E-08	4.05782E-05
1400	9.62943E+05	4.86337E+04	5.87450E+04	3.87925E-04	4.77288E-08	4.15144E-05
1450	9.63012E+05	4.85649E+04	5.87451E+04	3.87860E-04	3.22004E-08	4.24493E-05
1500	9.63081E+05	4.84963E+04	5.87451E+04	3.87796E-04	2.17241E-08	4.33827E-05
1550	9.63149E+05	4.84278E+04	5.87452E+04	3.87731E-04	1.46562E-08	4.43149E-05
1600	9.63217E+05	4.83594E+04	5.87452E+04	3.87666E-04	9.88778E-09	4.52457E-05
1650	9.63286E+05	4.82913E+04	5.87453E+04	3.87602E-04	6.67079E-09	4.61752E-05
1700	9.63354E+05	4.82232E+04	5.87453E+04	3.87537E-04	4.50044E-09	4.71033E-05
1750	9.63422E+05	4.81553E+04	5.87454E+04	3.87473E-04	3.03621E-09	4.80301E-05
1800	9.63489E+05	4.80876E+04	5.87454E+04	3.87409E-04	2.04837E-09	4.89556E-05
1850	9.63557E+05	4.80200E+04	5.87455E+04	3.87345E-04	1.38193E-09	4.98798E-05

1900	9.63624E+05	4.79526E+04	5.87456E+04	3.87281E-04	9.32311E-10	5.08026E-05
1950	9.63692E+05	4.78853E+04	5.87456E+04	3.87217E-04	6.28979E-10	5.17242E-05
2000	9.63759E+05	4.78182E+04	5.87457E+04	3.87153E-04	4.24337E-10	5.26445E-05
2050	9.63826E+05	4.77512E+04	5.87457E+04	3.87089E-04	2.86276E-10	5.35634E-05
2100	9.63893E+05	4.76844E+04	5.87458E+04	3.87026E-04	1.93134E-10	5.44811E-05
2150	9.63959E+05	4.76177E+04	5.87458E+04	3.86963E-04	1.30296E-10	5.53975E-05
2200	9.64026E+05	4.75512E+04	5.87459E+04	3.86899E-04	8.79032E-11	5.63126E-05
2250	9.64092E+05	4.74848E+04	5.87459E+04	3.86836E-04	5.93030E-11	5.72264E-05
2300	9.64158E+05	4.74185E+04	5.87460E+04	3.86773E-04	4.00082E-11	5.81389E-05
2350	9.64224E+05	4.73524E+04	5.87460E+04	3.86710E-04	2.69911E-11	5.90502E-05
2400	9.64290E+05	4.72865E+04	5.87461E+04	3.86647E-04	1.82092E-11	5.99601E-05
2450	9.64356E+05	4.72206E+04	5.87461E+04	3.86584E-04	1.22846E-11	6.08689E-05
2500	9.64422E+05	4.71550E+04	5.87462E+04	3.86522E-04	8.28764E-12	6.17764E-05
2550	9.64487E+05	4.70895E+04	5.87463E+04	3.86459E-04	5.59114E-12	6.26826E-05
2600	9.64553E+05	4.70241E+04	5.87463E+04	3.86397E-04	3.77198E-12	6.35876E-05
2650	9.64618E+05	4.69589E+04	5.87464E+04	3.86334E-04	2.54471E-12	6.44913E-05
2700	9.64683E+05	4.68938E+04	5.87464E+04	3.86272E-04	1.71674E-12	6.53938E-05
2750	9.64748E+05	4.68288E+04	5.87465E+04	3.86210E-04	1.15817E-12	6.62950E-05
2800	9.64813E+05	4.67640E+04	5.87465E+04	3.86148E-04	7.81339E-13	6.71950E-05
2850	9.64877E+05	4.66993E+04	5.87466E+04	3.86085E-04	5.27116E-13	6.80938E-05
2900	9.64942E+05	4.66348E+04	5.87466E+04	3.86023E-04	3.55609E-13	6.89914E-05
2950	9.65006E+05	4.65704E+04	5.87467E+04	3.85962E-04	2.39904E-13	6.98877E-05
3000	9.65071E+05	4.65062E+04	5.87467E+04	3.85900E-04	1.61846E-13	7.07828E-05
3050	9.65135E+05	4.64420E+04	5.87468E+04	3.85838E-04	1.09186E-13	7.16767E-05
3100	9.65198E+05	4.63781E+04	5.87468E+04	3.85776E-04	7.36600E-14	7.25694E-05
3150	9.65262E+05	4.63142E+04	5.87469E+04	3.85715E-04	4.96930E-14	7.34609E-05
3200	9.65326E+05	4.62505E+04	5.87469E+04	3.85653E-04	3.35242E-14	7.43512E-05
3250	9.65389E+05	4.61870E+04	5.87470E+04	3.85592E-04	2.26163E-14	7.52403E-05
3300	9.65453E+05	4.61236E+04	5.87470E+04	3.85531E-04	1.52575E-14	7.61282E-05
3350	9.65516E+05	4.60603E+04	5.87471E+04	3.85469E-04	1.02931E-14	7.70149E-05
3400	9.65579E+05	4.59971E+04	5.87471E+04	3.85408E-04	6.94395E-15	7.79004E-05
3450	9.65642E+05	4.59341E+04	5.87472E+04	3.85347E-04	4.68454E-15	7.87847E-05
3500	9.65705E+05	4.58712E+04	5.87473E+04	3.85286E-04	3.16029E-15	7.96679E-05
3550	9.65768E+05	4.58085E+04	5.87473E+04	3.85225E-04	2.13200E-15	8.05499E-05
3600	9.65830E+05	4.57458E+04	5.87474E+04	3.85164E-04	1.43829E-15	8.14307E-05
3650	9.65892E+05	4.56834E+04	5.87474E+04	3.85103E-04	9.70300E-16	8.23103E-05
3700	9.65955E+05	4.56210E+04	5.87475E+04	3.85042E-04	6.54583E-16	8.31888E-05
3750	9.66017E+05	4.55588E+04	5.87475E+04	3.84982E-04	4.41594E-16	8.40661E-05
3800	9.66079E+05	4.54967E+04	5.87476E+04	3.84921E-04	2.97907E-16	8.49423E-05
3850	9.66141E+05	4.54348E+04	5.87476E+04	3.84860E-04	2.00973E-16	8.58173E-05
3900	9.66203E+05	4.53730E+04	5.87477E+04	3.84800E-04	1.35580E-16	8.66912E-05

3950	9.66264E+05	4.53113E+04	5.87478E+04	3.84739E-04	9.14641E-17	8.75639E-05
4000	9.66326E+05	4.52497E+04	5.87478E+04	3.84679E-04	6.17030E-17	8.84355E-05
4050	9.66387E+05	4.51883E+04	5.87479E+04	3.84619E-04	4.16257E-17	8.93059E-05
4100	9.66448E+05	4.51270E+04	5.87479E+04	3.84558E-04	2.80813E-17	9.01752E-05
4150	9.66509E+05	4.50658E+04	5.87480E+04	3.84498E-04	1.89440E-17	9.10434E-05
4200	9.66570E+05	4.50048E+04	5.87480E+04	3.84438E-04	1.27798E-17	9.19104E-05
4250	9.66631E+05	4.49439E+04	5.87481E+04	3.84378E-04	8.62142E-18	9.27764E-05
4300	9.66692E+05	4.48831E+04	5.87481E+04	3.84318E-04	5.81610E-18	9.36412E-05
4350	9.66752E+05	4.48225E+04	5.87482E+04	3.84258E-04	3.92360E-18	9.45049E-05
4400	9.66813E+05	4.47620E+04	5.87482E+04	3.84198E-04	2.64690E-18	9.53675E-05
4450	9.66873E+05	4.47016E+04	5.87483E+04	3.84139E-04	1.78562E-18	9.62289E-05
4500	9.66933E+05	4.46413E+04	5.87484E+04	3.84079E-04	1.20459E-18	9.70893E-05
4550	9.66994E+05	4.45811E+04	5.87484E+04	3.84019E-04	8.12627E-19	9.79486E-05
4600	9.67053E+05	4.45211E+04	5.87485E+04	3.83960E-04	5.48204E-19	9.88067E-05
4650	9.67113E+05	4.44612E+04	5.87485E+04	3.83900E-04	3.69821E-19	9.96638E-05
4700	9.67173E+05	4.44015E+04	5.87486E+04	3.83841E-04	2.49483E-19	1.00520E-04
4750	9.67233E+05	4.43418E+04	5.87486E+04	3.83781E-04	1.68303E-19	1.01375E-04
4800	9.67292E+05	4.42823E+04	5.87487E+04	3.83722E-04	1.13538E-19	1.02228E-04
4850	9.67351E+05	4.42229E+04	5.87487E+04	3.83662E-04	7.65928E-20	1.03081E-04
4900	9.67411E+05	4.41636E+04	5.87488E+04	3.83603E-04	5.16697E-20	1.03933E-04
4950	9.67470E+05	4.41045E+04	5.87488E+04	3.83544E-04	3.48565E-20	1.04783E-04
5000	9.67529E+05	4.40455E+04	5.87489E+04	3.83485E-04	2.35142E-20	1.05633E-04
5050	9.67587E+05	4.39866E+04	5.87490E+04	3.83426E-04	1.58627E-20	1.06481E-04
5100	9.67646E+05	4.39278E+04	5.87490E+04	3.83367E-04	1.07010E-20	1.07329E-04
5150	9.67705E+05	4.38691E+04	5.87491E+04	3.83308E-04	7.21887E-21	1.08175E-04
5200	9.67763E+05	4.38106E+04	5.87491E+04	3.83249E-04	4.86984E-21	1.09020E-04
5250	9.67822E+05	4.37522E+04	5.87492E+04	3.83190E-04	3.28518E-21	1.09864E-04
5300	9.67880E+05	4.36939E+04	5.87492E+04	3.83132E-04	2.21617E-21	1.10708E-04
5350	9.67938E+05	4.36357E+04	5.87493E+04	3.83073E-04	1.49502E-21	1.11550E-04
5400	9.67996E+05	4.35777E+04	5.87493E+04	3.83014E-04	1.00854E-21	1.12391E-04
5450	9.68054E+05	4.35197E+04	5.87494E+04	3.82956E-04	6.80354E-22	1.13231E-04
5500	9.68112E+05	4.34619E+04	5.87494E+04	3.82897E-04	4.58963E-22	1.14070E-04
5550	9.68169E+05	4.34042E+04	5.87495E+04	3.82839E-04	3.09614E-22	1.14908E-04
5600	9.68227E+05	4.33466E+04	5.87495E+04	3.82780E-04	2.08863E-22	1.15744E-04
5650	9.68284E+05	4.32892E+04	5.87496E+04	3.82722E-04	1.40898E-22	1.16580E-04
5700	9.68341E+05	4.32318E+04	5.87496E+04	3.82664E-04	9.50484E-23	1.17415E-04
5750	9.68399E+05	4.31746E+04	5.87497E+04	3.82605E-04	6.41188E-23	1.18249E-04
5800	9.68456E+05	4.31175E+04	5.87498E+04	3.82547E-04	4.32539E-23	1.19082E-04
5850	9.68513E+05	4.30605E+04	5.87498E+04	3.82489E-04	2.91787E-23	1.19914E-04
5900	9.68569E+05	4.30036E+04	5.87499E+04	3.82431E-04	1.96836E-23	1.20744E-04
5950	9.68626E+05	4.29468E+04	5.87499E+04	3.82373E-04	1.32784E-23	1.21574E-04

6000	9.68683E+05	4.28902E+04	5.87500E+04	3.82315E-04	8.95742E-24	1.22403E-04
6050	9.68739E+05	4.28337E+04	5.87500E+04	3.82257E-04	6.04256E-24	1.23231E-04
6100	9.68795E+05	4.27772E+04	5.87501E+04	3.82199E-04	4.07623E-24	1.24057E-04
6150	9.68852E+05	4.27209E+04	5.87501E+04	3.82142E-04	2.74977E-24	1.24883E-04
6200	9.68908E+05	4.26648E+04	5.87502E+04	3.82084E-04	1.85496E-24	1.25708E-04
6250	9.68964E+05	4.26087E+04	5.87502E+04	3.82026E-04	1.25133E-24	1.26532E-04
6300	9.69020E+05	4.25527E+04	5.87503E+04	3.81969E-04	8.44124E-25	1.27354E-04
6350	9.69076E+05	4.24969E+04	5.87503E+04	3.81911E-04	5.69433E-25	1.28176E-04
6400	9.69131E+05	4.24411E+04	5.87504E+04	3.81854E-04	3.84130E-25	1.28997E-04
6450	9.69187E+05	4.23855E+04	5.87504E+04	3.81796E-04	2.59127E-25	1.29817E-04
6500	9.69242E+05	4.23300E+04	5.87505E+04	3.81739E-04	1.74802E-25	1.30635E-04
6550	9.69298E+05	4.22746E+04	5.87505E+04	3.81682E-04	1.17918E-25	1.31453E-04
6600	9.69353E+05	4.22193E+04	5.87506E+04	3.81624E-04	7.95455E-26	1.32270E-04
6650	9.69408E+05	4.21641E+04	5.87506E+04	3.81567E-04	5.36598E-26	1.33086E-04
6700	9.69463E+05	4.21091E+04	5.87507E+04	3.81510E-04	3.61978E-26	1.33901E-04
6750	9.69518E+05	4.20541E+04	5.87507E+04	3.81453E-04	2.44183E-26	1.34715E-04
6800	9.69573E+05	4.19993E+04	5.87508E+04	3.81396E-04	1.64720E-26	1.35528E-04
6850	9.69627E+05	4.19445E+04	5.87509E+04	3.81339E-04	1.11117E-26	1.36340E-04
6900	9.69682E+05	4.18899E+04	5.87509E+04	3.81282E-04	7.49566E-27	1.37151E-04
6950	9.69736E+05	4.18354E+04	5.87510E+04	3.81225E-04	5.05640E-27	1.37961E-04
7000	9.69791E+05	4.17810E+04	5.87510E+04	3.81168E-04	3.41092E-27	1.38771E-04
7050	9.69845E+05	4.17267E+04	5.87511E+04	3.81111E-04	2.30092E-27	1.39579E-04
7100	9.69899E+05	4.16725E+04	5.87511E+04	3.81055E-04	1.55214E-27	1.40386E-04
7150	9.69953E+05	4.16184E+04	5.87512E+04	3.80998E-04	1.04704E-27	1.41193E-04
7200	9.70007E+05	4.15644E+04	5.87512E+04	3.80941E-04	7.06302E-28	1.41998E-04
7250	9.70061E+05	4.15105E+04	5.87513E+04	3.80885E-04	4.76452E-28	1.42802E-04
7300	9.70114E+05	4.14568E+04	5.87513E+04	3.80828E-04	3.21401E-28	1.43606E-04
7350	9.70168E+05	4.14031E+04	5.87514E+04	3.80772E-04	2.16808E-28	1.44409E-04
7400	9.70222E+05	4.13496E+04	5.87514E+04	3.80715E-04	1.46252E-28	1.45210E-04
7450	9.70275E+05	4.12961E+04	5.87515E+04	3.80659E-04	9.86575E-29	1.46011E-04
7500	9.70328E+05	4.12428E+04	5.87515E+04	3.80603E-04	6.65514E-29	1.46811E-04
7550	9.70381E+05	4.11895E+04	5.87516E+04	3.80546E-04	4.48935E-29	1.47610E-04
7600	9.70434E+05	4.11364E+04	5.87516E+04	3.80490E-04	3.02837E-29	1.48408E-04
7650	9.70488E+05	4.10834E+04	5.87517E+04	3.80434E-04	2.04284E-29	1.49205E-04
7700	9.70540E+05	4.10305E+04	5.87517E+04	3.80378E-04	1.37804E-29	1.50001E-04
7750	9.70593E+05	4.09776E+04	5.87518E+04	3.80322E-04	9.29577E-30	1.50796E-04
7800	9.70646E+05	4.09249E+04	5.87518E+04	3.80266E-04	6.27061E-30	1.51591E-04
7850	9.70698E+05	4.08723E+04	5.87519E+04	3.80210E-04	4.22994E-30	1.52384E-04
7900	9.70751E+05	4.08198E+04	5.87519E+04	3.80154E-04	2.85337E-30	1.53177E-04
7950	9.70803E+05	4.07674E+04	5.87520E+04	3.80098E-04	1.92478E-30	1.53969E-04
8000	9.70855E+05	4.07151E+04	5.87520E+04	3.80042E-04	1.29839E-30	1.54759E-04

8050	9.70908E+05	4.06629E+04	5.87521E+04	3.79987E-04	8.75844E-31	1.55549E-04
8100	9.70959E+05	4.06108E+04	5.87521E+04	3.79931E-04	5.90811E-31	1.56338E-04
8150	9.71011E+05	4.05588E+04	5.87522E+04	3.79875E-04	3.98539E-31	1.57126E-04
8200	9.71063E+05	4.05069E+04	5.87522E+04	3.79820E-04	2.68839E-31	1.57913E-04
8250	9.71115E+05	4.04551E+04	5.87523E+04	3.79764E-04	1.81348E-31	1.58700E-04
8300	9.71167E+05	4.04034E+04	5.87523E+04	3.79709E-04	1.22330E-31	1.59485E-04
8350	9.71218E+05	4.03518E+04	5.87524E+04	3.79653E-04	8.25191E-32	1.60270E-04
8400	9.71270E+05	4.03004E+04	5.87524E+04	3.79598E-04	5.56640E-32	1.61054E-04
8450	9.71321E+05	4.02490E+04	5.87525E+04	3.79543E-04	3.75486E-32	1.61836E-04
8500	9.71372E+05	4.01977E+04	5.87525E+04	3.79487E-04	2.53287E-32	1.62618E-04
8550	9.71423E+05	4.01465E+04	5.87526E+04	3.79432E-04	1.70857E-32	1.63399E-04
8600	9.71474E+05	4.00954E+04	5.87526E+04	3.79377E-04	1.15253E-32	1.64180E-04
8650	9.71525E+05	4.00444E+04	5.87527E+04	3.79322E-04	7.77444E-33	1.64959E-04
8700	9.71576E+05	3.99935E+04	5.87527E+04	3.79267E-04	5.24429E-33	1.65737E-04
8750	9.71627E+05	3.99427E+04	5.87528E+04	3.79212E-04	3.53756E-33	1.66515E-04
8800	9.71677E+05	3.98920E+04	5.87528E+04	3.79157E-04	2.38628E-33	1.67292E-04
8850	9.71728E+05	3.98414E+04	5.87529E+04	3.79102E-04	1.60967E-33	1.68068E-04
8900	9.71778E+05	3.97909E+04	5.87529E+04	3.79047E-04	1.08581E-33	1.68843E-04
8950	9.71829E+05	3.97405E+04	5.87530E+04	3.78992E-04	7.32437E-34	1.69617E-04
9000	9.71879E+05	3.96902E+04	5.87530E+04	3.78937E-04	4.94067E-34	1.70390E-04
9050	9.71929E+05	3.96400E+04	5.87531E+04	3.78882E-04	3.33274E-34	1.71163E-04
9100	9.71979E+05	3.95898E+04	5.87531E+04	3.78828E-04	2.24810E-34	1.71934E-04
9150	9.72029E+05	3.95398E+04	5.87532E+04	3.78773E-04	1.51646E-34	1.72705E-04
9200	9.72079E+05	3.94899E+04	5.87532E+04	3.78718E-04	1.02293E-34	1.73475E-04
9250	9.72129E+05	3.94401E+04	5.87533E+04	3.78664E-04	6.90015E-35	1.74244E-04
9300	9.72178E+05	3.93903E+04	5.87533E+04	3.78609E-04	4.65449E-35	1.75013E-04
9350	9.72228E+05	3.93407E+04	5.87534E+04	3.78555E-04	3.13968E-35	1.75780E-04
9400	9.72277E+05	3.92911E+04	5.87534E+04	3.78500E-04	2.11786E-35	1.76547E-04
9450	9.72327E+05	3.92417E+04	5.87535E+04	3.78446E-04	1.42860E-35	1.77312E-04
9500	9.72376E+05	3.91923E+04	5.87535E+04	3.78392E-04	9.63657E-36	1.78077E-04
9550	9.72425E+05	3.91431E+04	5.87536E+04	3.78337E-04	6.50031E-36	1.78842E-04
9600	9.72474E+05	3.90939E+04	5.87536E+04	3.78283E-04	4.38476E-36	1.79605E-04
9650	9.72523E+05	3.90448E+04	5.87537E+04	3.78229E-04	2.95772E-36	1.80368E-04
9700	9.72572E+05	3.89958E+04	5.87537E+04	3.78175E-04	1.99511E-36	1.81129E-04
9750	9.72621E+05	3.89469E+04	5.87538E+04	3.78121E-04	1.34579E-36	1.81890E-04
9800	9.72670E+05	3.88981E+04	5.87538E+04	3.78067E-04	9.07794E-37	1.82650E-04
9850	9.72718E+05	3.88494E+04	5.87539E+04	3.78013E-04	6.12346E-37	1.83410E-04
9900	9.72767E+05	3.88008E+04	5.87539E+04	3.77959E-04	4.13053E-37	1.84168E-04
9950	9.72815E+05	3.87523E+04	5.87539E+04	3.77905E-04	2.78622E-37	1.84926E-04
10000	9.72864E+05	3.87039E+04	5.87540E+04	3.77851E-04	1.87942E-37	1.85683E-04

APPENDIX B: INPUT FILES USED FOR PANEL CRA-2014 PA CALCULATIONS

B.1 GM_PANEL_CRA14.INP

```
!-------------------------------------------------------------
! Analysis    : CRA-2014 PA Calculation (CRA14) AP-164
! Analysis ID : CRA14
! Remark      : This input file is unchanged from previous
!             : analyses. See original description below.
!-------------------------------------------------------------
!=============================================================================
!   FILETYPE: GENMESH input text file
!   TITLE: Simple GENMESH to set up Source Term CDB
!   ANALYSTS: Christine Stockman
!   DATE: May 31, 1996
!=============================================================================
!
  *SETUP
    DIM=     3
    ORIGIN= 0.0, 0.0, 0.0
    IJKMAX= 2, 2, 2
  *GRID
!   ==================== X direction ======================
    DEL, COORD=X, DEL=   1.00, INRANGE=  1,  2, FACTOR= 1.0
!   ==================== Y direction ======================
    DEL, COORD=Y, DEL=   1.00, INRANGE=  1,  2, FACTOR= 1.0
!   ==================== Z direction ======================
    DEL, COORD=Z, DEL=   1.00, INRANGE=  1,  2, FACTOR= 1.0
!
  *REGIONS
   REGION= 1, IRANGE= 1,2, JRANGE= 1,2 KRANGE= 1, 2
 !=============================================================================
  *END
```

B.2 MS_PANEL_CRA14.INP

```
!=============================================================================
! TITLE:    MATSET input file for PANEL (CRA14-BV for SOURCE term in PANEL runs)
!  This input file is for the 2014 CRA Calculation (AP-164)
! ANALYSTS: S. KIM
! CREATED:  February 11, 2013
! A modification of the 2009 PABC Source Term MATSET input file
! PURPOSE:  PREPARE INPUT CDB FOR  PANEL
!=============================================================================
!
*HEADING
 RUN=0
 SCALE=SOURCE
 SCENARIO=00
 TITLE=SOURCE TERM
!
*PRINT_ASSIGNED_VALUES
!
*UNITS=SI
!
*CREATE_BLOCK
  BLOCKID=      2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, &
           16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, &
           31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, &
           46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, &
           61, 62, 63, 64, 65
*RETRIEVE*NAME
 COORDINATE, DIM=3, NAMES=X, Y, Z
 MATERIAL,    1=GLOBAL, 2=REFCON, &
    3=AM241,  4=AM243,  5=CF252,  6=CM243,  7=CM244,  8=CM245, &
    9=CM248, 10=CS137, 11=NP237, 12=PA231, 13=PB210, 14=PM147, &
   15=PU238, 16=PU239, 17=PU240, 18=PU241, 19=PU242, 20=PU244, &
```

```
   21=RA226, 22=RA228, 23=SR90,  24=TH229, 25=TH230, 26=TH232, &
   27=U233,  28=U234,  29=U235,  30=U236,  31=U238,  &
   32=AM, 33=CF, 34=CM, 35=CS, 36=NP, 37=PA, 38=PB, 39=PM, 40=PU, &
   41=RA, 42=SR, 43=TH, 44=U,  &
   45=SOLMOD3, 46=SOLMOD4, 47=SOLMOD5, 48=SOLMOD6, &
   49=PHUMOX3, 50=PHUMOX4, 51=PHUMOX5, 52=PHUMOX6, &
   53=SOLAM3,  54=SOLPU3,  55=SOLPU4,  56=SOLTH4,  57=SOLU4,  58=SOLU6, &
   59=AM241L, 60=PU238L, 61=PU239L, 62=TH230L, 63=U234L,  64=BOREHOLE, &
   65=WAS_AREA
!MATERIALS 59-63 ARE LUMPED PARAMETERS FOR NUTS
!
 PROPERTY   MATERIAL=WAS_AREA,  NAMES =PROBDEG
 PROPERTY   MATERIAL=Global,    NAMES =OXSTAT,DBRMINBV
 PROPERTY   MATERIAL=REFCON,    NAMES =YRSEC,VPANLEX,VREPOS
!ISOTOPES
 PROPERTY   MATERIAL=Am241,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Am243,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cf252,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm243,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm244,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm245,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm248,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cs137,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Np237,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pa231,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pb210,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pm147,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu238,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu239,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu240,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu241,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu242,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu244,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Ra226,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Ra228,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Sr90 ,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Th229,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Th230,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Th232,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U233,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U234,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U235,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U236,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U238,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
!LUMPED ISOTOPES
 PROPERTY   MATERIAL=AM241L,    NAMES =InvCHD,InvRHD
 PROPERTY   MATERIAL=PU238L,    NAMES =InvCHD,InvRHD
 PROPERTY   MATERIAL=PU239L,    NAMES =InvCHD,InvRHD
 PROPERTY   MATERIAL=TH230L,    NAMES =InvCHD,InvRHD
 PROPERTY   MATERIAL=U234L,     NAMES =InvCHD,InvRHD
!ELEMENTS
 PROPERTY   MATERIAL=AM,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=NP,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=PU,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=TH,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=U,         NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
!OXIDATION STATES
 PROPERTY   MATERIAL=SOLMOD3,   NAMES
=SOLSOH,SOLCOH,SOLSOH2,SOLCOH2,SOLSOH3,SOLCOH3,SOLSOH4,SOLCOH4,SOLSOH5,SOLCOH5,SOLVAR
 PROPERTY   MATERIAL=SOLMOD4,   NAMES
=SOLSOH,SOLCOH,SOLSOH2,SOLCOH2,SOLSOH3,SOLCOH3,SOLSOH4,SOLCOH4,SOLSOH5,SOLCOH5,SOLVAR
 PROPERTY   MATERIAL=SOLMOD5,   NAMES
=SOLSOH,SOLCOH,SOLSOH2,SOLCOH2,SOLSOH3,SOLCOH3,SOLSOH4,SOLCOH4,SOLSOH5,SOLCOH5
 PROPERTY   MATERIAL=SOLMOD6,   NAMES =SOLSOH,SOLCOH
 PROPERTY   MATERIAL=PHUMOX3,   NAMES =PHUMSIM,PHUMCIM
 PROPERTY   MATERIAL=PHUMOX4,   NAMES =PHUMSIM,PHUMCIM
 PROPERTY   MATERIAL=PHUMOX5,   NAMES =PHUMSIM,PHUMCIM
 PROPERTY   MATERIAL=PHUMOX6,   NAMES =PHUMSIM,PHUMCIM
!WASTE UNIT FACTOR
 PROPERTY   MATERIAL=BOREHOLE,  NAMES=WUF
!==========================================================================
```

```
*END
!-----------------------------------------------------------------------
```

B.3 ALG1_PANEL_CRA14.INP

```
!
! This input file is for the CRA14 calculatioon, AP-164
! This file calculates the total moles of U,Pu, and Th and the mole fractions
! of U233+U234, PU238, and TH229+TH230, as well as the maximun mole fractions
!
ALLTIMES
U_MOLE  = SDMU233/ATWEIGHT[27]+SDMU234/ATWEIGHT[28]+SDMU235/ATWEIGHT[29]+ &
          SDMU236/ATWEIGHT[30]+SDMU238/ATWEIGHT[31]
PU_MOLE = SDMPU238/ATWEIGHT[15]+SDMPU239/ATWEIGHT[16]+SDMPU240/ATWEIGHT[17]+ &
          SDMPU241/ATWEIGHT[18]+SDMPU242/ATWEIGHT[19]+SDMPU244/ATWEIGHT[20]
TH_MOLE = SDMTH229/ATWEIGHT[24]+SDMTH230/ATWEIGHT[25]+SDMTH232/ATWEIGHT[26]

MF_U  = (SDMU233/ATWEIGHT[27]+SDMU234/ATWEIGHT[28])/U_MOLE
MF_PU = SDMPU238/ATWEIGHT[15]/PU_MOLE
MF_TH = (SDMTH229/ATWEIGHT[24]+SDMTH230/ATWEIGHT[25])/TH_MOLE

LSD_U  = -LOG10(ENVMAX(MF_U))
LSD_PU = -LOG10(ENVMAX(MF_PU))
LSD_TH = -LOG10(ENVMAX(MF_TH))

EXIT
```

B.4.1 ALG2_PANEL_CRA14BV1.INP

```
!
! This input file is for the CRA14-BV Calculation, AP-164
! Sets the maximum over time of the Log Sol Difference
! 1x brine volume
!
STEP 201

DELETE HISTORY

LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])

LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])

LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! COMPUTE SCALEING FOR ONE PANEL AND PANEL MIN BRINE VOLUME
LIMIT BLOCK 2
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE*1.0)

EXIT
```

B.4.2 ALG2_PANEL_CRA14BV2.INP

```
!
! This input file is for the CRA14-BV Calculation, AP-164
! Sets the maximum over time of the Log Sol Difference
! 2x brine volume
!
STEP 201

DELETE HISTORY

LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])
```

```
LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])

LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! COMPUTE SCALEING FOR ONE PANEL AND PANEL MIN BRINE VOLUME
LIMIT BLOCK 2
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE*2.0)

EXIT
```

B.4.3 ALG2_PANEL_CRA14BV3.INP

```
!
! This input file is for the CRA14-BV Calculation, AP-164
! Sets the maximum over time of the Log Sol Difference
! 3x brine volume
!
STEP 201

DELETE HISTORY

LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])

LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])

LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! COMPUTE SCALEING FOR ONE PANEL AND PANEL MIN BRINE VOLUME
LIMIT BLOCK 2
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE*3.0)

EXIT
```

B.4.4 ALG2_PANEL_CRA14BV4.INP

```
!
! This input file is for the CRA14-BV Calculation, AP-164
! Sets the maximum over time of the Log Sol Difference
! 4x brine volume
!
STEP 201

DELETE HISTORY

LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])

LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])

LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! COMPUTE SCALEING FOR ONE PANEL AND PANEL MIN BRINE VOLUME
LIMIT BLOCK 2
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE*4.0)

EXIT
```

B.4.5 ALG2_PANEL_CRA14BV5.INP

```
!
! This input file is for the CRA14-BV Calculation, AP-164
! Sets the maximum over time of the Log Sol Difference
! 5x brine volume
!
STEP 201

DELETE HISTORY

LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])

LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])

LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! COMPUTE SCALEING FOR ONE PANEL AND PANEL MIN BRINE VOLUME
LIMIT BLOCK 2
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE*5.0)

EXIT
```

B.5.1 ALG3_PANEL_CRA14BV1.INP

```
!
! This input file is for the CRA14-BV Calculations, AP-164
! 1x brine volume
!
! NOW, DEFINE SOLS AND SOLC
!
LIMIT BLOCK 45 ! (SOLMOD3)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
LIMIT BLOCK 46 ! (SOLMOD4)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
LIMIT BLOCK 47 ! (SOLMOD5)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
LIMIT BLOCK 48 ! (SOLMOD6)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
!PROPOGATE THE SOLUBILITY VARIABILITY TO VARIABLES NEEDED FOR PANEL
!
LIMIT BLOCK 53 ! (SOLAM3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 54 ! (SOLPU3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 55 ! (SOLPU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 57 ! (SOLU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
```

```
LIMIT BLOCK 56 ! (SOLTH4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 58 ! (SOLU6)
SOLSIM=MAKEPROP(0.)
SOLCIM=MAKEPROP(0.)
!
! SET HALFLIFE AND ATWEIGHT FOR AM241L SAME AS FOR AM241
!
LIMIT BLOCK 59 ! (AM241L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:3])
HALFLIFE=MAKEPROP(HALFLIFE[B:3])
!
! SET HALFLIFE AND ATWEIGHT FOR PU238L SAME AS FOR PU238
!
LIMIT BLOCK 60 ! (PU238L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:15])
HALFLIFE=MAKEPROP(HALFLIFE[B:15])
!
! SET HALFLIFE AND ATWEIGHT FOR PU239L SAME AS FOR PU239
!
LIMIT BLOCK 61 ! (PU239L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:16])
HALFLIFE=MAKEPROP(HALFLIFE[B:16])
!
! SET HALFLIFE AND ATWEIGHT FOR TH230L SAME AS FOR TH230
!
LIMIT BLOCK 62 ! (TH230L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:25])
HALFLIFE=MAKEPROP(HALFLIFE[B:25])
!
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
END
```

B.5.2 ALG3_PANEL_CRA14BV2.INP

```
!
! This input file is for the CRA14-BV Calculations, AP-164
! 2x brine volume
!
! NOW, DEFINE SOLS AND SOLC
!
LIMIT BLOCK 45 ! (SOLMOD3)
SOLS=MAKEPROP(SOLSOH2)
SOLC=MAKEPROP(SOLCOH2)
!
LIMIT BLOCK 46 ! (SOLMOD4)
SOLS=MAKEPROP(SOLSOH2)
SOLC=MAKEPROP(SOLCOH2)
!
LIMIT BLOCK 47 ! (SOLMOD5)
SOLS=MAKEPROP(SOLSOH2)
SOLC=MAKEPROP(SOLCOH2)
!
LIMIT BLOCK 48 ! (SOLMOD6)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
!PROPOGATE THE SOLUBILITY VARIABILITY TO VARIABLES NEEDED FOR PANEL
!
LIMIT BLOCK 53 ! (SOLAM3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
```

```
LIMIT BLOCK 54 ! (SOLPU3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 55 ! (SOLPU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 57 ! (SOLU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 56 ! (SOLTH4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 58 ! (SOLU6)
SOLSIM=MAKEPROP(0.)
SOLCIM=MAKEPROP(0.)
!
! SET HALFLIFE AND ATWEIGHT FOR AM241L SAME AS FOR AM241
!
LIMIT BLOCK 59 ! (AM241L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:3])
HALFLIFE=MAKEPROP(HALFLIFE[B:3])
!
! SET HALFLIFE AND ATWEIGHT FOR PU238L SAME AS FOR PU238
!
LIMIT BLOCK 60 ! (PU238L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:15])
HALFLIFE=MAKEPROP(HALFLIFE[B:15])
!
! SET HALFLIFE AND ATWEIGHT FOR PU239L SAME AS FOR PU239
!
LIMIT BLOCK 61 ! (PU239L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:16])
HALFLIFE=MAKEPROP(HALFLIFE[B:16])
!
! SET HALFLIFE AND ATWEIGHT FOR TH230L SAME AS FOR TH230
!
LIMIT BLOCK 62 ! (TH230L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:25])
HALFLIFE=MAKEPROP(HALFLIFE[B:25])
!
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
END
```

B.5.3 ALG3_PANEL_CRA14BV3.INP

```
!
! This input file is for the CRA14-BV Calculations, AP-164
! 3x brine volume
!
! NOW, DEFINE SOLS AND SOLC
!
LIMIT BLOCK 45 ! (SOLMOD3)
SOLS=MAKEPROP(SOLSOH3)
SOLC=MAKEPROP(SOLCOH3)
!
LIMIT BLOCK 46 ! (SOLMOD4)
SOLS=MAKEPROP(SOLSOH3)
SOLC=MAKEPROP(SOLCOH3)
!
LIMIT BLOCK 47 ! (SOLMOD5)
SOLS=MAKEPROP(SOLSOH3)
```

```
SOLC=MAKEPROP(SOLCOH3)
!
LIMIT BLOCK 48 ! (SOLMOD6)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
!PROPOGATE THE SOLUBILITY VARIABILITY TO VARIABLES NEEDED FOR PANEL
!
LIMIT BLOCK 53 ! (SOLAM3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 54 ! (SOLPU3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 55 ! (SOLPU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 57 ! (SOLU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 56 ! (SOLTH4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 58 ! (SOLU6)
SOLSIM=MAKEPROP(0.)
SOLCIM=MAKEPROP(0.)
!
! SET HALFLIFE AND ATWEIGHT FOR AM241L SAME AS FOR AM241
!
LIMIT BLOCK 59 ! (AM241L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:3])
HALFLIFE=MAKEPROP(HALFLIFE[B:3])
!
! SET HALFLIFE AND ATWEIGHT FOR PU238L SAME AS FOR PU238
!
LIMIT BLOCK 60 ! (PU238L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:15])
HALFLIFE=MAKEPROP(HALFLIFE[B:15])
!
! SET HALFLIFE AND ATWEIGHT FOR PU239L SAME AS FOR PU239
!
LIMIT BLOCK 61 ! (PU239L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:16])
HALFLIFE=MAKEPROP(HALFLIFE[B:16])
!
! SET HALFLIFE AND ATWEIGHT FOR TH230L SAME AS FOR TH230
!
LIMIT BLOCK 62 ! (TH230L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:25])
HALFLIFE=MAKEPROP(HALFLIFE[B:25])
!
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
END
```

B.5.4 ALG3_PANEL_CRA14BV4.INP

```
!
! This input file is for the CRA14-BV Calculations, AP-164
! 4x brine volume
!
```

```
! NOW, DEFINE SOLS AND SOLC
!
LIMIT BLOCK 45 ! (SOLMOD3)
SOLS=MAKEPROP(SOLSOH4)
SOLC=MAKEPROP(SOLCOH4)
!
LIMIT BLOCK 46 ! (SOLMOD4)
SOLS=MAKEPROP(SOLSOH4)
SOLC=MAKEPROP(SOLCOH4)
!
LIMIT BLOCK 47 ! (SOLMOD5)
SOLS=MAKEPROP(SOLSOH4)
SOLC=MAKEPROP(SOLCOH4)
!
LIMIT BLOCK 48 ! (SOLMOD6)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
!PROPOGATE THE SOLUBILITY VARIABILITY TO VARIABLES NEEDED FOR PANEL
!
LIMIT BLOCK 53 ! (SOLAM3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 54 ! (SOLPU3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 55 ! (SOLPU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 57 ! (SOLU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 56 ! (SOLTH4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 58 ! (SOLU6)
SOLSIM=MAKEPROP(0.)
SOLCIM=MAKEPROP(0.)
!
! SET HALFLIFE AND ATWEIGHT FOR AM241L SAME AS FOR AM241
!
LIMIT BLOCK 59 ! (AM241L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:3])
HALFLIFE=MAKEPROP(HALFLIFE[B:3])
!
! SET HALFLIFE AND ATWEIGHT FOR PU238L SAME AS FOR PU238
!
LIMIT BLOCK 60 ! (PU238L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:15])
HALFLIFE=MAKEPROP(HALFLIFE[B:15])
!
! SET HALFLIFE AND ATWEIGHT FOR PU239L SAME AS FOR PU239
!
LIMIT BLOCK 61 ! (PU239L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:16])
HALFLIFE=MAKEPROP(HALFLIFE[B:16])
!
! SET HALFLIFE AND ATWEIGHT FOR TH230L SAME AS FOR TH230
!
LIMIT BLOCK 62 ! (TH230L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:25])
HALFLIFE=MAKEPROP(HALFLIFE[B:25])
!
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
```

```
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
END
```

B.5.5 ALG3_PANEL_CRA14BV5.INP

```
!
! This input file is for the CRA14-BV Calculations, AP-164
! 5x brine volume
!
! NOW, DEFINE SOLS AND SOLC
!
LIMIT BLOCK 45 ! (SOLMOD3)
SOLS=MAKEPROP(SOLSOH5)
SOLC=MAKEPROP(SOLCOH5)
!
LIMIT BLOCK 46 ! (SOLMOD4)
SOLS=MAKEPROP(SOLSOH5)
SOLC=MAKEPROP(SOLCOH5)
!
LIMIT BLOCK 47 ! (SOLMOD5)
SOLS=MAKEPROP(SOLSOH5)
SOLC=MAKEPROP(SOLCOH5)
!
LIMIT BLOCK 48 ! (SOLMOD6)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
!PROPOGATE THE SOLUBILITY VARIABILITY TO VARIABLES NEEDED FOR PANEL
!
LIMIT BLOCK 53 ! (SOLAM3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 54 ! (SOLPU3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 55 ! (SOLPU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 57 ! (SOLU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 56 ! (SOLTH4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 58 ! (SOLU6)
SOLSIM=MAKEPROP(0.)
SOLCIM=MAKEPROP(0.)
!
! SET HALFLIFE AND ATWEIGHT FOR AM241L SAME AS FOR AM241
!
LIMIT BLOCK 59 ! (AM241L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:3])
HALFLIFE=MAKEPROP(HALFLIFE[B:3])
!
! SET HALFLIFE AND ATWEIGHT FOR PU238L SAME AS FOR PU238
!
LIMIT BLOCK 60 ! (PU238L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:15])
HALFLIFE=MAKEPROP(HALFLIFE[B:15])
!
! SET HALFLIFE AND ATWEIGHT FOR PU239L SAME AS FOR PU239
!
LIMIT BLOCK 61 ! (PU239L)
```

```
ATWEIGHT=MAKEPROP(ATWEIGHT[B:16])
HALFLIFE=MAKEPROP(HALFLIFE[B:16])
!
! SET HALFLIFE AND ATWEIGHT FOR TH230L SAME AS FOR TH230
!
LIMIT BLOCK 62 ! (TH230L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:25])
HALFLIFE=MAKEPROP(HALFLIFE[B:25])
!
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
END
```

B.6 LHS3_DUMMY.INP

```
This file is not read by LHS3, but its presence is required.


[End of file]
```